



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2016 – 12:28 AM GMT

PDB ID : 4YPB  
Title : Precleavage 70S structure of the *P. vulgaris* HigB DeltaH92 toxin bound to the AAA codon  
Authors : Schureck, M.A.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.  
Deposited on : 2015-03-12  
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

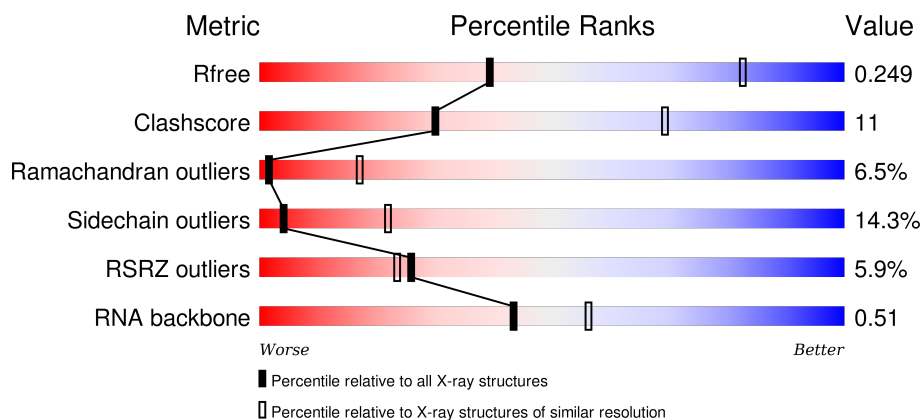
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1476 (3.50-3.30)                                      |
| Clashscore            | 102246                      | 1611 (3.50-3.30)                                      |
| Ramachandran outliers | 100387                      | 1571 (3.50-3.30)                                      |
| Sidechain outliers    | 100360                      | 1571 (3.50-3.30)                                      |
| RSRZ outliers         | 91569                       | 1485 (3.50-3.30)                                      |
| RNA backbone          | 2183                        | 1041 (4.00-2.80)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | QA    | 1522   | <div> <div>3%</div> <div>55%</div> <div>33%</div> <div>10%</div> <div>..</div> </div> |
| 1   | XA    | 1522   | <div> <div>3%</div> <div>55%</div> <div>34%</div> <div>9%</div> <div>..</div> </div>  |
| 2   | QB    | 256    | <div> <div>11%</div> <div>52%</div> <div>31%</div> <div>8%</div> <div>8%</div> </div> |
| 2   | XB    | 256    | <div> <div>8%</div> <div>50%</div> <div>34%</div> <div>8%</div> <div>8%</div> </div>  |

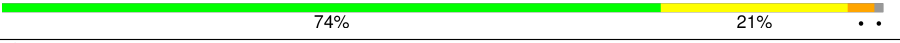





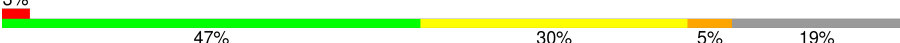
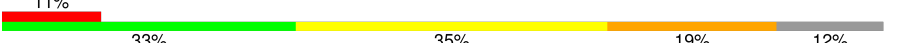
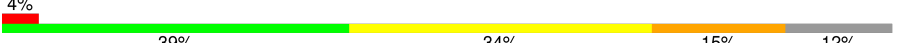


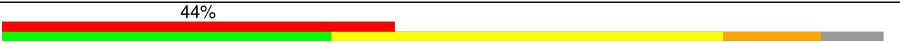
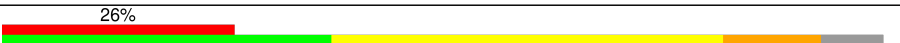








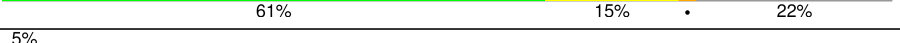



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | QC    | 239    |                  |
| 3   | XC    | 239    |                  |
| 4   | QD    | 209    |                  |
| 4   | XD    | 209    |                  |
| 5   | QE    | 162    |                  |
| 5   | XE    | 162    |                  |
| 6   | QF    | 101    |                  |
| 6   | XF    | 101    |                  |
| 7   | QG    | 156    |                  |
| 7   | XG    | 156    |                  |
| 8   | QH    | 138    |                  |
| 8   | XH    | 138    |                  |
| 9   | QI    | 128    |                  |
| 9   | XI    | 128    |                  |
| 10  | QJ    | 105    |                  |
| 10  | XJ    | 105    |                  |
| 11  | QK    | 129    |                  |
| 11  | XK    | 129    |                  |
| 12  | QL    | 132    |                  |
| 12  | XL    | 132    |                  |
| 13  | QM    | 126    |                  |
| 13  | XM    | 126    |                  |
| 14  | QN    | 61     |                  |
| 14  | XN    | 61     |                  |
| 15  | QO    | 89     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 15  | XO    | 89     |    |
| 16  | QP    | 88     |    |
| 16  | XP    | 88     |    |
| 17  | QQ    | 105    |    |
| 17  | XQ    | 105    |    |
| 18  | QR    | 88     |    |
| 18  | XR    | 88     |    |
| 19  | QS    | 93     |    |
| 19  | XS    | 93     |    |
| 20  | QT    | 106    |    |
| 20  | XT    | 106    |    |
| 21  | QU    | 27     |    |
| 21  | XU    | 27     |  |
| 22  | QV    | 77     |  |
| 22  | QW    | 77     |  |
| 22  | XV    | 77     |  |
| 22  | XW    | 77     |  |
| 23  | QX    | 25     |  |
| 23  | XX    | 25     |  |
| 24  | QY    | 117    |  |
| 24  | XY    | 117    |  |
| 25  | RA    | 2916   |  |
| 25  | YA    | 2916   |  |
| 26  | RB    | 124    |  |
| 26  | YB    | 124    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27  | RD    | 276    |                  |
| 27  | YD    | 276    |                  |
| 28  | RE    | 206    |                  |
| 28  | YE    | 206    |                  |
| 29  | RF    | 210    |                  |
| 29  | YF    | 210    |                  |
| 30  | RG    | 182    |                  |
| 30  | YG    | 182    |                  |
| 31  | RH    | 180    |                  |
| 31  | YH    | 180    |                  |
| 32  | RI    | 148    |                  |
| 32  | YI    | 148    |                  |
| 33  | RN    | 140    |                  |
| 33  | YN    | 140    |                  |
| 34  | RO    | 122    |                  |
| 34  | YO    | 122    |                  |
| 35  | RP    | 150    |                  |
| 35  | YP    | 150    |                  |
| 36  | RQ    | 141    |                  |
| 36  | YQ    | 141    |                  |
| 37  | RR    | 118    |                  |
| 37  | YR    | 118    |                  |
| 38  | RS    | 112    |                  |
| 38  | YS    | 112    |                  |
| 39  | RT    | 146    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39  | YT    | 146    |                  |
| 40  | RU    | 118    |                  |
| 40  | YU    | 118    |                  |
| 41  | RV    | 101    |                  |
| 41  | YV    | 101    |                  |
| 42  | RW    | 113    |                  |
| 42  | YW    | 113    |                  |
| 43  | RX    | 96     |                  |
| 43  | YX    | 96     |                  |
| 44  | RY    | 110    |                  |
| 44  | YY    | 110    |                  |
| 45  | RZ    | 206    |                  |
| 45  | YZ    | 206    |                  |
| 46  | R0    | 85     |                  |
| 46  | Y0    | 85     |                  |
| 47  | R1    | 98     |                  |
| 47  | Y1    | 98     |                  |
| 48  | R2    | 72     |                  |
| 48  | Y2    | 72     |                  |
| 49  | R3    | 60     |                  |
| 49  | Y3    | 60     |                  |
| 50  | R4    | 71     |                  |
| 50  | Y4    | 71     |                  |
| 51  | R5    | 60     |                  |
| 51  | Y5    | 60     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52  | R6    | 54     |                  |
| 52  | Y6    | 54     |                  |
| 53  | R7    | 49     |                  |
| 53  | Y7    | 49     |                  |
| 54  | R8    | 65     |                  |
| 54  | Y8    | 65     |                  |
| 55  | R9    | 37     |                  |
| 55  | Y9    | 37     |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | QA    | 1601 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1604 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1605 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1606 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1608 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1609 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1619 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1625 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1632 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1636 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1637 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1639 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1640 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1641 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1643 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1644 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1645 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1651 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1656 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1662 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1668 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1670 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1681 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | QA    | 1682 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1687 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1699 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1703 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1719 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1728 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1729 | -         | -        | -       | X                |
| 56  | MG   | QA    | 1741 | -         | -        | -       | X                |
| 56  | MG   | R5    | 102  | -         | -        | -       | X                |
| 56  | MG   | RA    | 3001 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3002 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3004 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3007 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3011 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3012 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3013 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3014 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3018 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3022 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3026 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3027 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3028 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3032 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3033 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3034 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3037 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3039 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3045 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3047 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3048 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3050 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3051 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3053 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3055 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3056 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3057 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3061 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3063 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3065 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3066 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3067 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3071 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | RA    | 3072 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3073 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3074 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3079 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3080 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3081 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3082 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3083 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3094 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3095 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3099 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3103 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3104 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3105 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3107 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3108 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3110 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3116 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3125 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3128 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3131 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3135 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3140 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3148 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3149 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3153 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3155 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3159 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3165 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3166 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3173 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3177 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3184 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3189 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3193 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3195 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3197 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3198 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3202 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3205 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3206 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3209 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | RA    | 3213 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3222 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3225 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3228 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3233 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3244 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3247 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3251 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3254 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3259 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3263 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3264 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3275 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3291 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3292 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3295 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3296 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3306 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3316 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3318 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3331 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3339 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3343 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3350 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3355 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3357 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3363 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3365 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3368 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3369 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3370 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3376 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3377 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3385 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3386 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3405 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3407 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3411 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3420 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3425 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3427 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3430 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | RA    | 3431 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3432 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3434 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3436 | -         | -        | -       | X                |
| 56  | MG   | RA    | 3438 | -         | -        | -       | X                |
| 56  | MG   | RD    | 302  | -         | -        | -       | X                |
| 56  | MG   | RQ    | 202  | -         | -        | -       | X                |
| 56  | MG   | XA    | 1601 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1604 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1605 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1607 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1611 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1613 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1618 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1624 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1625 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1635 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1638 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1640 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1643 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1644 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1650 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1652 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1659 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1664 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1667 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1692 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1695 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1697 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1701 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1717 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1742 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1745 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1754 | -         | -        | -       | X                |
| 56  | MG   | XA    | 1755 | -         | -        | -       | X                |
| 56  | MG   | Y1    | 101  | -         | -        | -       | X                |
| 56  | MG   | YA    | 3003 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3006 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3010 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3011 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3012 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3013 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | YA    | 3017 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3018 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3025 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3026 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3027 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3031 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3033 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3038 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3042 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3044 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3049 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3054 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3055 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3056 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3060 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3062 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3064 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3066 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3070 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3071 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3072 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3073 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3078 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3079 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3080 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3081 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3082 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3088 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3092 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3097 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3099 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3101 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3102 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3103 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3106 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3109 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3111 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3121 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3122 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3127 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3130 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3133 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | YA    | 3137 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3146 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3147 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3151 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3155 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3156 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3167 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3170 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3186 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3190 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3191 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3192 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3201 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3203 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3204 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3208 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3209 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3210 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3220 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3221 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3224 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3227 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3233 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3234 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3240 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3249 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3250 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3255 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3264 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3276 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3280 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3282 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3295 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3305 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3325 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3335 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3336 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3338 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3339 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3340 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3375 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3392 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | YA    | 3407 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3414 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3416 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3418 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3424 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3425 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3426 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3428 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3431 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3455 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3459 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3460 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3463 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3467 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3472 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3473 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3484 | -         | -        | -       | X                |
| 56  | MG   | YA    | 3485 | -         | -        | -       | X                |
| 56  | MG   | YD    | 301  | -         | -        | -       | X                |
| 56  | MG   | YF    | 301  | -         | -        | -       | X                |
| 56  | MG   | YQ    | 201  | -         | -        | -       | X                |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 297549 atoms, of which 18 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | QA    | 1511     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32472 | 14453 | 6011 | 10497 | 1511 |         |         |       |
| 1   | XA    | 1508     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32409 | 14425 | 6001 | 10475 | 1508 |         |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | QB    | 236      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1915  | 1223 | 343 | 344 | 5 |         |         |       |
| 2   | XB    | 236      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1915  | 1223 | 343 | 344 | 5 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | QC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |
| 3   | XC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | QD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |
| 4   | XD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | QE    | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1178  | 743 | 221 | 210 | 4 |         |         |       |
| 5   | XE    | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1178  | 743 | 221 | 210 | 4 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | QF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 6   | XF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | QG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 7   | XG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | QH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 8   | XH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | QI    | 128      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1018  | 644 | 198 | 175 | 1 |         |         |       |
| 9   | XI    | 128      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1018  | 644 | 198 | 175 | 1 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | QJ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 801   | 504 | 157 | 139 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | XJ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 801   | 504 | 157 | 139 | 1 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | QK    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 901   | 560 | 171 | 167 | 3 |         |         |       |
| 11  | XK    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 901   | 560 | 171 | 167 | 3 |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | QL    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 975   | 614 | 196 | 164 | 1 |         |         |       |
| 12  | XL    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 975   | 614 | 196 | 164 | 1 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | QM    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 937   | 579 | 193 | 163 | 2 |         |         |       |
| 13  | XM    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 937   | 579 | 193 | 163 | 2 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | QN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 14  | XN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | QO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |
| 15  | XO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | QP    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |
| 16  | XP    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | QQ    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |
| 17  | XQ    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | QR    | 71       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 585   | 373 | 116 | 96 |         |         |       |
| 18  | XR    | 71       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 585   | 373 | 116 | 96 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | QS    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 656   | 419 | 121 | 114 | 2 |         |         |       |
| 19  | XS    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 656   | 419 | 121 | 114 | 2 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | QT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |
| 20  | XT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

- Molecule 21 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | QU    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |
| 21  | XU    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |

- Molecule 22 is a RNA chain called tRNA fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | QV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |
| 22  | QW    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |
| 22  | XV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |
| 22  | XW    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 297 | 535 | 76 |         |         |       |

- Molecule 23 is a RNA chain called messenger RNA.

| Mol | Chain | Residues | Atoms |     |   |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---|----|-----|----|---------|---------|-------|
| 23  | QX    | 20       | Total | C   | H | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 449   | 199 | 9 | 89 | 132 | 20 |         |         |       |
| 23  | XX    | 20       | Total | C   | H | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 449   | 199 | 9 | 89 | 132 | 20 |         |         |       |

- Molecule 24 is a protein called Host inhibition of growth B.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 24  | QY    | 91       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 746   | 478 | 131 | 137 |         |         |       |
| 24  | XY    | 91       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 746   | 478 | 131 | 137 |         |         |       |

There are 54 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| QY    | 0       | MET      | -      | initiating methionine | UNP Q7A225 |
| QY    | 1       | GLY      | -      | expression tag        | UNP Q7A225 |
| QY    | 92      | LYS      | -      | expression tag        | UNP Q7A225 |
| QY    | 93      | LEU      | -      | expression tag        | UNP Q7A225 |
| QY    | 94      | GLY      | -      | expression tag        | UNP Q7A225 |
| QY    | 95      | PRO      | -      | expression tag        | UNP Q7A225 |
| QY    | 96      | GLU      | -      | expression tag        | UNP Q7A225 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| QY    | 97      | GLN      | -      | expression tag        | UNP Q7A225 |
| QY    | 98      | LYS      | -      | expression tag        | UNP Q7A225 |
| QY    | 99      | LEU      | -      | expression tag        | UNP Q7A225 |
| QY    | 100     | ILE      | -      | expression tag        | UNP Q7A225 |
| QY    | 101     | SER      | -      | expression tag        | UNP Q7A225 |
| QY    | 102     | GLU      | -      | expression tag        | UNP Q7A225 |
| QY    | 103     | GLU      | -      | expression tag        | UNP Q7A225 |
| QY    | 104     | ASP      | -      | expression tag        | UNP Q7A225 |
| QY    | 105     | LEU      | -      | expression tag        | UNP Q7A225 |
| QY    | 106     | ASN      | -      | expression tag        | UNP Q7A225 |
| QY    | 107     | SER      | -      | expression tag        | UNP Q7A225 |
| QY    | 108     | ALA      | -      | expression tag        | UNP Q7A225 |
| QY    | 109     | VAL      | -      | expression tag        | UNP Q7A225 |
| QY    | 110     | ASP      | -      | expression tag        | UNP Q7A225 |
| QY    | 111     | HIS      | -      | expression tag        | UNP Q7A225 |
| QY    | 112     | HIS      | -      | expression tag        | UNP Q7A225 |
| QY    | 113     | HIS      | -      | expression tag        | UNP Q7A225 |
| QY    | 114     | HIS      | -      | expression tag        | UNP Q7A225 |
| QY    | 115     | HIS      | -      | expression tag        | UNP Q7A225 |
| QY    | 116     | HIS      | -      | expression tag        | UNP Q7A225 |
| XY    | 0       | MET      | -      | initiating methionine | UNP Q7A225 |
| XY    | 1       | GLY      | -      | expression tag        | UNP Q7A225 |
| XY    | 92      | LYS      | -      | expression tag        | UNP Q7A225 |
| XY    | 93      | LEU      | -      | expression tag        | UNP Q7A225 |
| XY    | 94      | GLY      | -      | expression tag        | UNP Q7A225 |
| XY    | 95      | PRO      | -      | expression tag        | UNP Q7A225 |
| XY    | 96      | GLU      | -      | expression tag        | UNP Q7A225 |
| XY    | 97      | GLN      | -      | expression tag        | UNP Q7A225 |
| XY    | 98      | LYS      | -      | expression tag        | UNP Q7A225 |
| XY    | 99      | LEU      | -      | expression tag        | UNP Q7A225 |
| XY    | 100     | ILE      | -      | expression tag        | UNP Q7A225 |
| XY    | 101     | SER      | -      | expression tag        | UNP Q7A225 |
| XY    | 102     | GLU      | -      | expression tag        | UNP Q7A225 |
| XY    | 103     | GLU      | -      | expression tag        | UNP Q7A225 |
| XY    | 104     | ASP      | -      | expression tag        | UNP Q7A225 |
| XY    | 105     | LEU      | -      | expression tag        | UNP Q7A225 |
| XY    | 106     | ASN      | -      | expression tag        | UNP Q7A225 |
| XY    | 107     | SER      | -      | expression tag        | UNP Q7A225 |
| XY    | 108     | ALA      | -      | expression tag        | UNP Q7A225 |
| XY    | 109     | VAL      | -      | expression tag        | UNP Q7A225 |
| XY    | 110     | ASP      | -      | expression tag        | UNP Q7A225 |
| XY    | 111     | HIS      | -      | expression tag        | UNP Q7A225 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| XY    | 112     | HIS      | -      | expression tag | UNP Q7A225 |
| XY    | 113     | HIS      | -      | expression tag | UNP Q7A225 |
| XY    | 114     | HIS      | -      | expression tag | UNP Q7A225 |
| XY    | 115     | HIS      | -      | expression tag | UNP Q7A225 |
| XY    | 116     | HIS      | -      | expression tag | UNP Q7A225 |

- Molecule 25 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 25  | RA    | 2891     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62269 | 27713 | 11649 | 20016 | 2891 |         |         |       |
| 25  | YA    | 2875     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61924 | 27560 | 11583 | 19906 | 2875 |         |         |       |

- Molecule 26 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26  | RB    | 122      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2617  | 1166 | 486 | 844 | 121 |         |         |       |
| 26  | YB    | 122      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2617  | 1166 | 486 | 844 | 121 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27  | RD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |
| 27  | YD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | RE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |
| 28  | YE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29  | RF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1627  | 1037 | 304 | 283 | 3 |         |         |       |
| 29  | YF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1627  | 1037 | 304 | 283 | 3 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | RG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |
| 30  | YG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | RH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |
| 31  | YH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | RI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |
| 32  | YI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | RN    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |
| 33  | YN    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | RO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | YO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | RP    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |
| 35  | YP    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | RQ    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 710 | 210 | 185 | 7 |         |         |       |
| 36  | YQ    | 139      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1107  | 707 | 209 | 184 | 7 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 37  | RR    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |  |         |         |       |
| 37  | YR    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |  |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 38  | RS    | 111      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |  |         |         |       |
| 38  | YS    | 111      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |  |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | RT    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |
| 39  | YT    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | RU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |
| 40  | YU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | RV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |
| 41  | YV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | RW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |
| 42  | YW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43  | RX    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |
| 43  | YX    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | RY    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |
| 44  | YY    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | RZ    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1404  | 897 | 252 | 252 | 3 |         |         |       |
| 45  | YZ    | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1461  | 933 | 260 | 265 | 3 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | R0    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 657   | 407 | 139 | 110 | 1 |         |         |       |
| 46  | Y0    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 657   | 407 | 139 | 110 | 1 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | R1    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |
| 47  | Y1    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | R2    | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 358 | 118 | 104 | 1 |         |         |       |
| 48  | Y2    | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 358 | 118 | 104 | 1 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49  | R3    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |
| 49  | Y3    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |

- Molecule 50 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | R4    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 573   | 359 | 107 | 103 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | Y4    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 573   | 359 | 107 | 103 | 4 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51  | R5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 51  | Y5    | 57       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 442   | 278 | 88 | 71 | 5 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | R6    | 48       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 68 | 4 |         |         |       |
| 52  | Y6    | 48       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 68 | 4 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53  | R7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |         |       |
| 53  | Y7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54  | R8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |
| 54  | Y8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 55  | R9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 55  | Y9    | 36       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 299   | 183 | 67 | 46 | 3 |         |         |       |

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | QA    | 150      | Total<br>150 | Mg<br>150 | 0       | 0       |
| 56  | YV    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | RP    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | QX    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | YA    | 487      | Total<br>487 | Mg<br>487 | 0       | 0       |
| 56  | Y5    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | YH    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | RT    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | QD    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | XS    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | Y1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | YD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | QV    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | YO    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | XA    | 163      | Total<br>163 | Mg<br>163 | 0       | 0       |
| 56  | YY    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | RQ    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | R0    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | QL    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | Y0    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | YG    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | YQ    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | RY    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | YN    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | XF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | RR    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | RD    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | R1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | XL    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | Y7    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | RV    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | R5    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | RA    | 441      | Total<br>441 | Mg<br>441 | 0       | 0       |
| 56  | YF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | YP    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | RE    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | R2    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | YB    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 56  | YW    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | XV    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | RB    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | XD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56  | RF    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 56  | YE    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

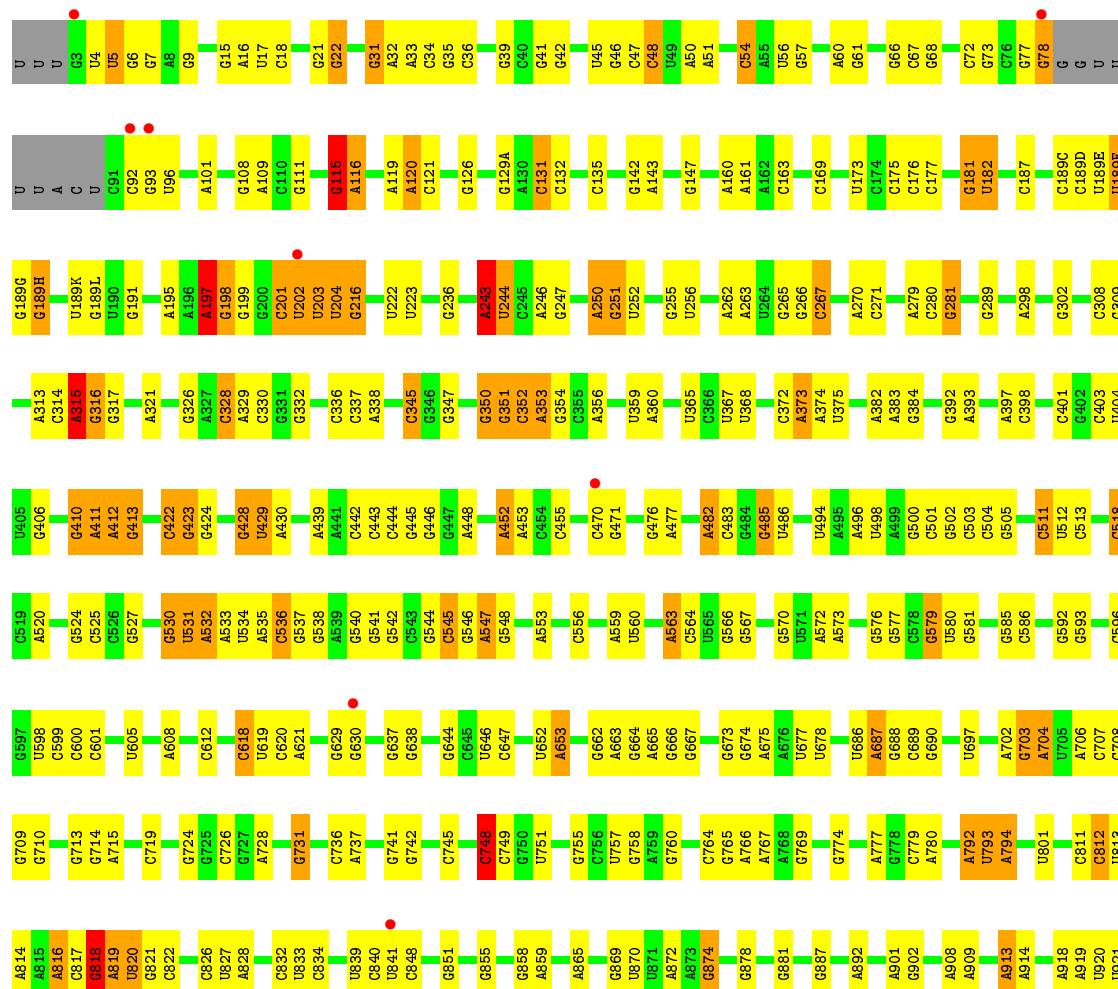
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57  | XD    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | QD    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | QN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | XN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

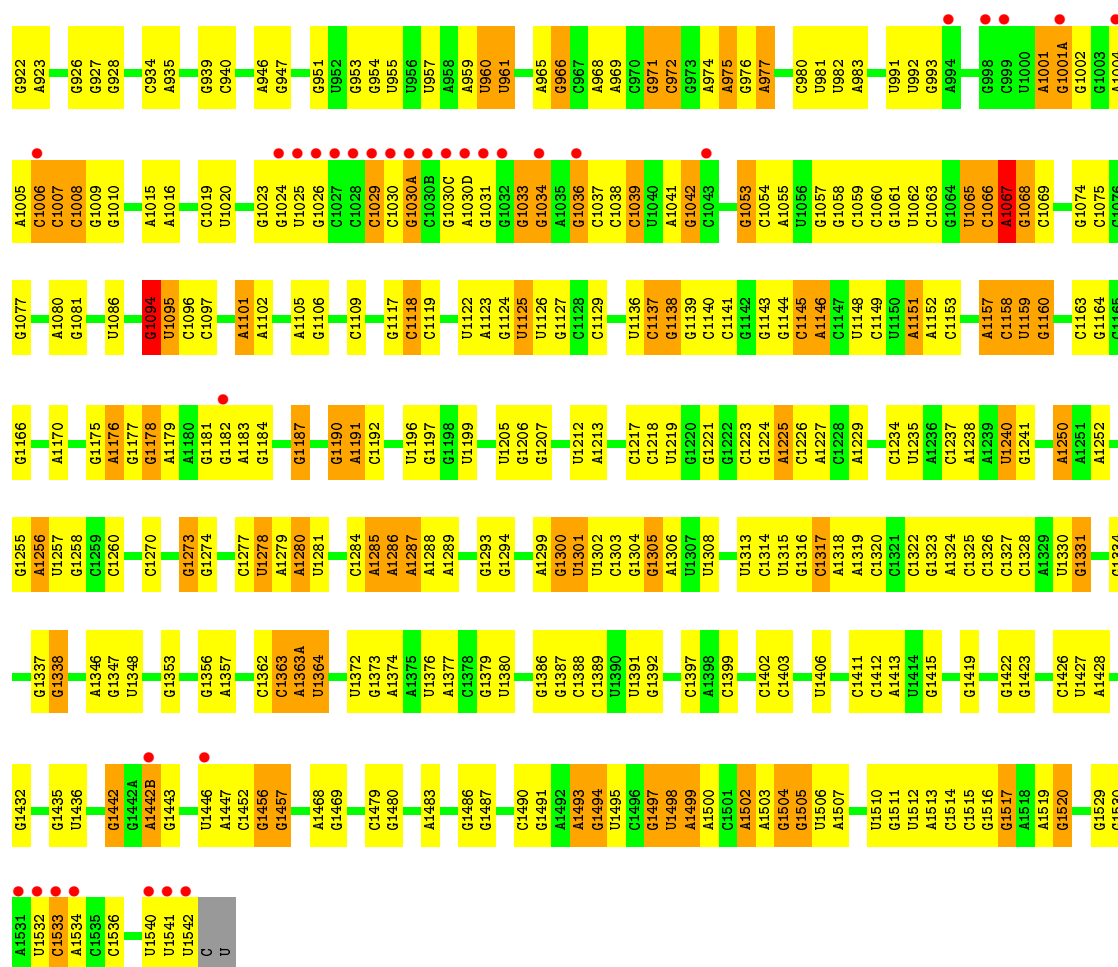
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Chain QA: 3% 55% 33% 10% 2%

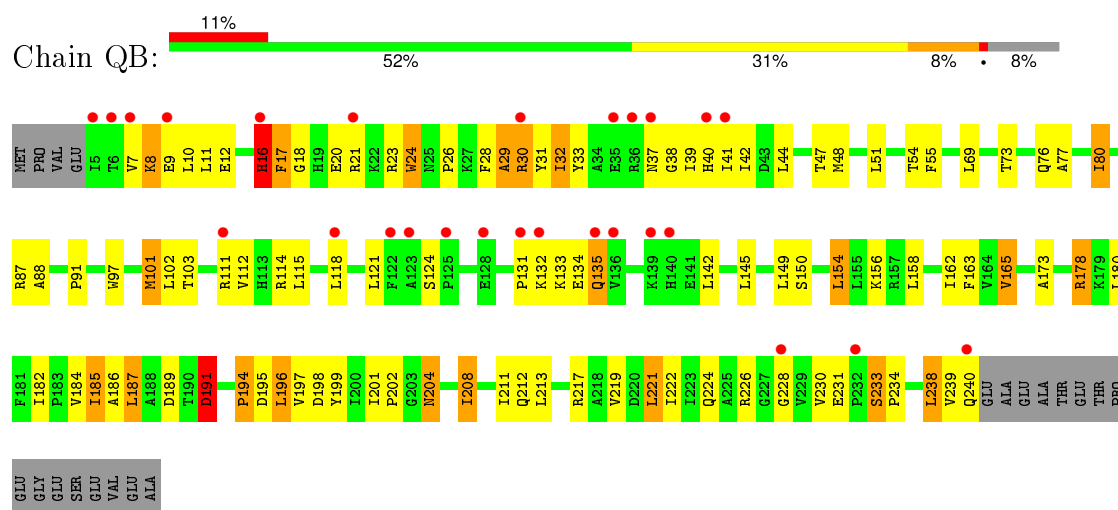
The visualization displays a sequence of 1024 QA pairs, categorized by color: Green (3%), Yellow (55%), Orange (33%), Red (10%), and Gray (2%). The pairs are arranged in a grid of 16 columns and 64 rows. Each pair is represented by a colored square containing a 4-digit hex code. The colors of the squares and the dots on the vertical bars to the left and right of the grid correspond to the QA type distribution shown in the bar chart at the top.

Hex codes visible in the grid include: G1021, G1022, G1023, G1024, G1025, G1026, C1027, C1028, C1029, C1030, G1030A, G1030B, G1030C, A1030D, G1031, G1032, G1033, G1034, A1035, G1036, C1037, G1038, G1039, A1040, G1042, C1045, C1051, G1052, G1053, G1054, A1055, G1056, G1057, G1058, C1059, C1060, G1061, G1062, C1063, G1065, A1067, G1068, C1069, G1070, G1071, A1004, A1005, C1006, C1007, C1008, G1009, A1014, G1081, U1086, G1087, G1094, G1095, G1096, G1097, G1098, G1099, G1100, G1101, G1102, G1103, G1104, G1105, G1106, G1107, G1108, G1109, G1110, G1111, G1112, G1113, G1114, G1115, G1116, G1117, G1118, G1119, G1120, G1121, G1122, G1123, G1124, G1125, G1126, G1127, G1128, G1129, G1130, G1131, G1132, G1133, G1134, G1135, G1136, G1137, G1138, G1139, G1140, G1141, G1142, G1143, G1144, G1145, G1146, G1147, G1148, G1149, G1150, G1151, G1152, G1153, G1154, G1155, G1156, G1157, G1158, G1159, G1160, G1161, G1162, G1163, G1164, G1165, G1166, G1167, G1168, G1169, G1170, G1171, G1172, G1173, G1174, G1175, G1176, G1177, G1178, G1179, G1180, G1181, G1182, G1183, G1184, G1185, G1186, G1187, G1188, G1189, G1190, G1191, G1192, G1193, G1194, G1195, G1196, G1197, G1198, G1199, G1200, G1201, G1202, G1203, G1204, G1205, G1206, G1207, G1208, G1209, G1210, G1211, G1212, G1213, G1214, G1215, G1216, G1217, G1218, G1219, G1220, G1221, G1222, G1223, G1224, G1225, G1226, G1227, G1228, G1229, G1230, G1231, G1232, G1233, G1234, G1235, G1236, G1237, G1238, G1239, G1240, G1241, G1242, G1243, G1244, G1245, G1246, G1247, G1248, G1249, G1250, G1251, G1252, G1253, G1254, G1255, G1256, G1257, G1258, G1259, G1260, G1261, G1262, G1263, G1264, G1265, G1266, G1267, G1268, G1269, G1270, G1271, G1272, G1273, G1274, G1275, G1276, G1277, G1278, G1279, G1280, G1281, G1282, G1283, G1284, G1285, G1286, G1287, G1288, G1289, G1290, G1291, G1292, G1293, G1294, G1295, G1296, G1297, G1298, G1299, G1300, G1301, G1302, G1303, G1304, G1305, G1306, G1307, G1308, G1309, G1310, G1311, G1312, G1313, G1314, G1315, G1316, G1317, G1318, G1319, G1320, G1321, G1322, G1323, G1324, G1325, G1326, G1327, G1328, G1329, G1330, G1331, G1332, G1333, G1334, G1335, G1336, G1337, G1338, G1339, G1340, G1341, G1342, G1343, G1344, G1345, G1346, G1347, G1348, G1349, G1350, G1351, G1352, G1353, G1354, G1355, G1356, G1357, G1358, G1359, G1360, G1361, G1362, G1363, G1364, G1365, G1366, G1367, G1368, G1369, G1370, G1371, G1372, G1373, G1374, G1375, G1376, G1377, G1378, G1379, G1380, G1381, G1382, G1383, G1384, G1385, G1386, G1387, G1388, G1389, G1390, G1391, G1392, G1393, G1394, G1395, G1396, G1397, G1398, G1399, G1400, G1401, G1402, G1403, G1404, G1405, G1406, G1407, G1408, G1409, G1410, G1411, G1412, G1413, G1414, G1415, G1416, G1417, G1418, G1419, G1420, G1421, G1422, G1423, G1424, G1425, G1426, G1427, G1428, G1429, G1430, G1431, G1432, G1433, G1434, G1435, G1436, G1437, G1438, G1439, G1440, G1441, G1442, G1443, G1444, G1445, G1446, G1447, G1448, G1449, G1450, G1451, G1452, G1453, G1454, G1455, G1456, G1457, G1458, G1459, G1460, G1461, G1462, G1463, G1464, G1465, G1466, G1467, G1468, G1469, G1470, G1471, G1472, G1473, G1474, G1475, G1476, G1477, G1478, G1479, G1480, G1481, G1482, G1483, G1484, G1485, G1486, G1487, G1488, G1489, G1490, G1491, G1492, G1493, G1494, G1495, G1496, G1497, G1498, G1499, G1500, G1501, G1502, G1503, G1504, G1505, G1506, G1507, G1508, G1509, G1510, G1511, G1512, G1513, G1514, G1515, G1516, G1517, G1518, G1519, G1520, G1521, G1522, G1523, G1524, G1525, G1526, G1527, G1528, G1529, G1530, G1531, G1532, G1533, G1534, G1535, G1536, G1537, G1538, G1539, G1540, G1541, G1542, G1543, G1544, G1545, G1546, G1547, G1548, G1549, G1550, G1551, G1552, G1553, G1554, G1555, G1556, G1557, G1558, G1559, G1560, G1561, G1562, G1563, G1564, G1565, G1566, G1567, G1568, G1569, G1570, G1571, G1572, G1573, G1574, G1575, G1576, G1577, G1578, G1579, G1580, G1581, G1582, G1583, G1584, G1585, G1586, G1587, G1588, G1589, G1590, G1591, G1592, G1593, G1594, G1595, G1596, G1597, G1598, G1599, G1600, G1601, G1602, G1603, G1604, G1605, G1606, G1607, G1608, G1609, G1610, G1611, G1612, G1613, G1614, G1615, G1616, G1617, G1618, G1619, G1620, G1621, G1622, G1623, G1624, G1625, G1626, G1627, G1628, G1629, G1630, G1631, G1632, G1633, G1634, G1635, G1636, G1637, G1638, G1639, G1640, G1641, G1642, G1643, G1644, G1645, G1646, G1647, G1648, G1649, G1650, G1651, G1652, G1653, G1654, G1655, G1656, G1657, G165



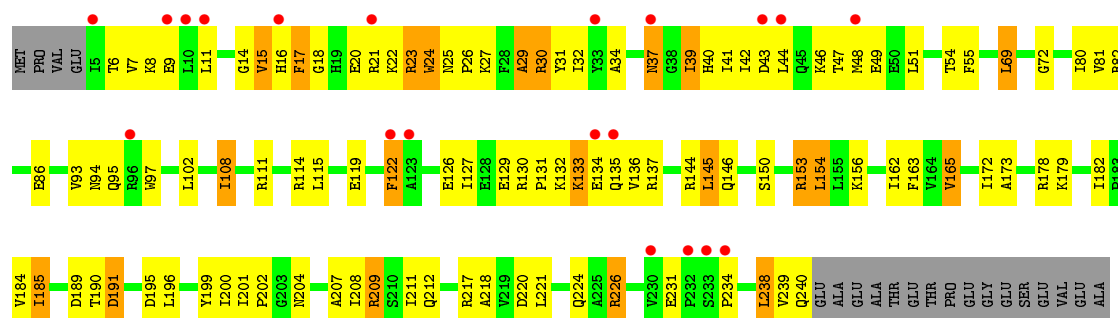


• Molecule 2: 30S ribosomal protein S2

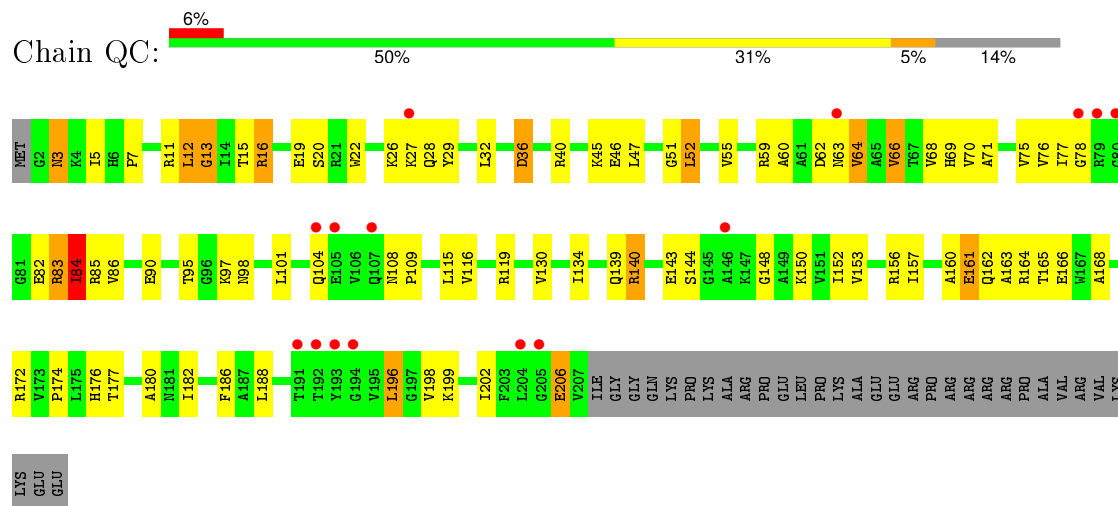


• Molecule 2: 30S ribosomal protein S2

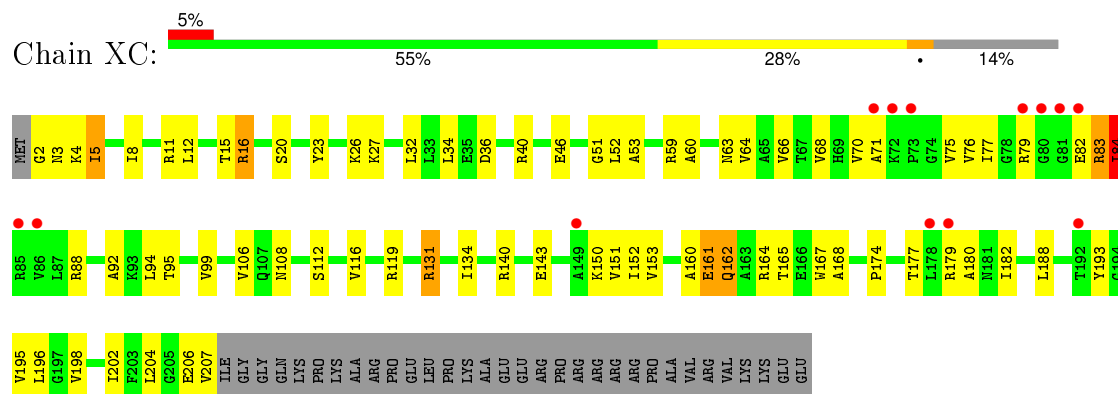




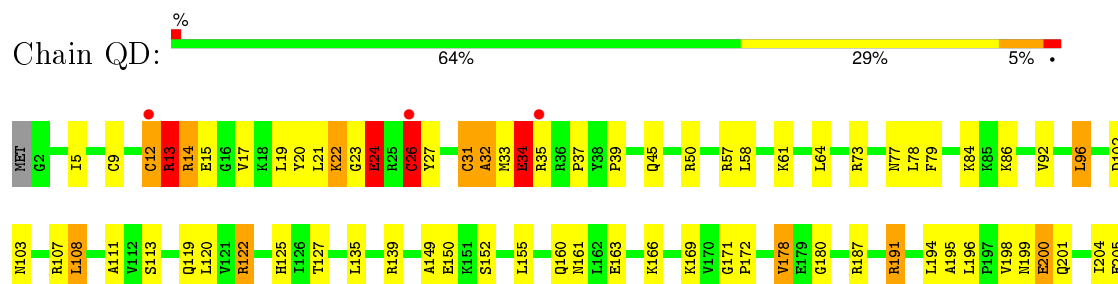
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

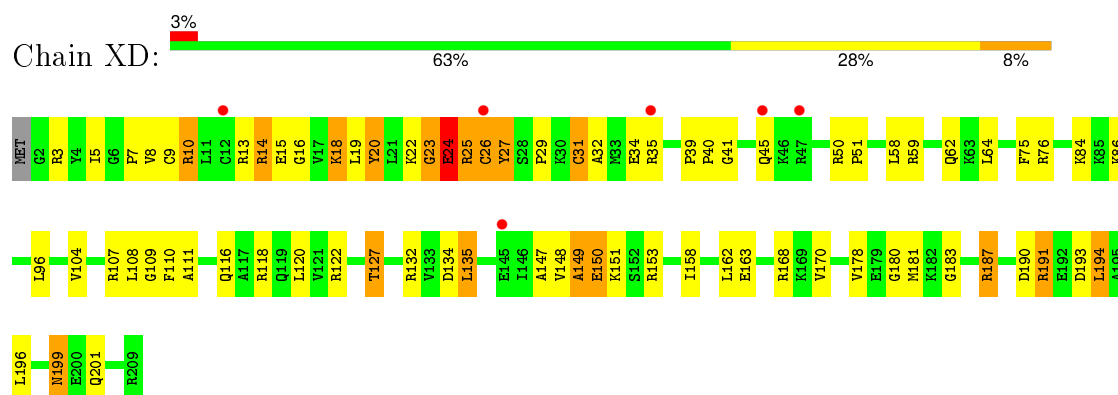


• Molecule 4: 30S ribosomal protein S4

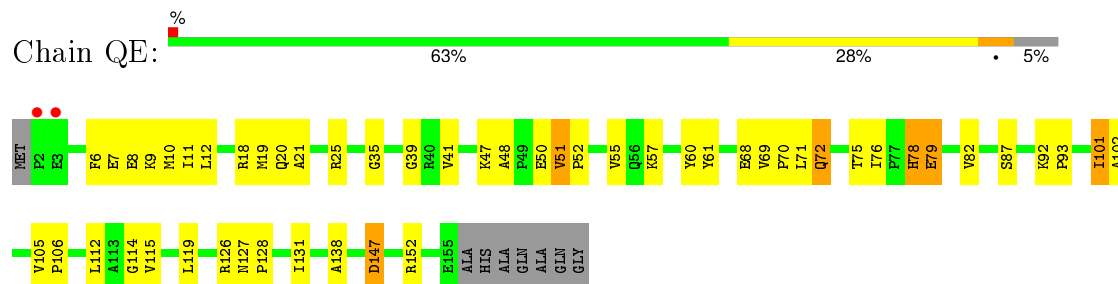




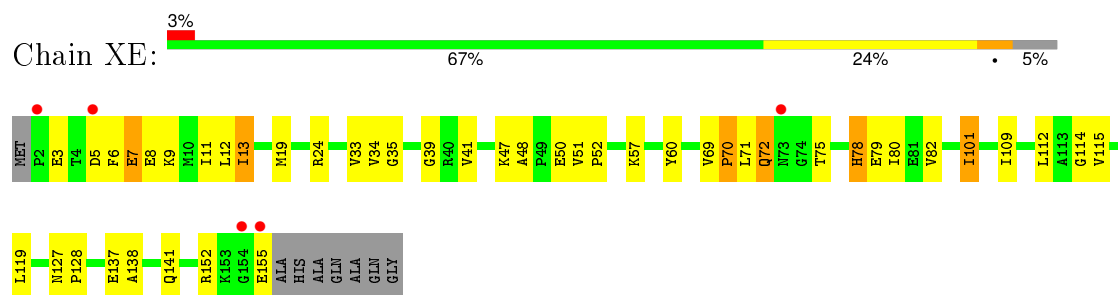
- Molecule 4: 30S ribosomal protein S4



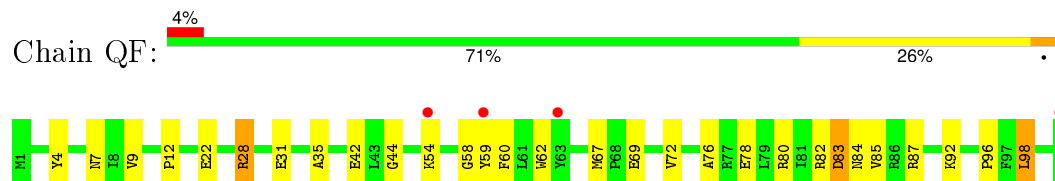
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5

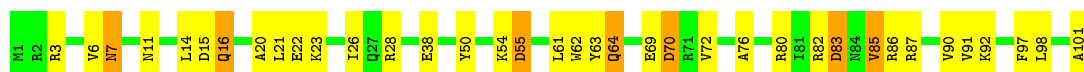


- Molecule 6: 30S ribosomal protein S6

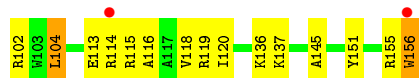


- Molecule 6: 30S ribosomal protein S6

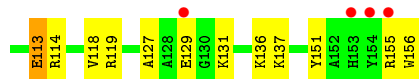




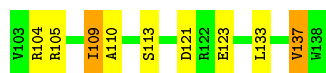
- Molecule 7: 30S ribosomal protein S7



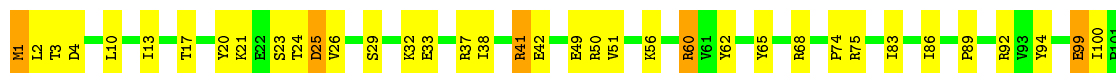
- Molecule 7: 30S ribosomal protein S7



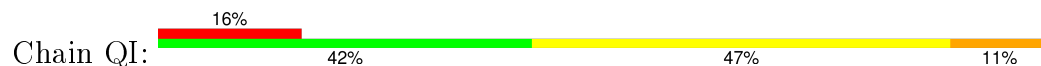
- Molecule 8: 30S ribosomal protein S8

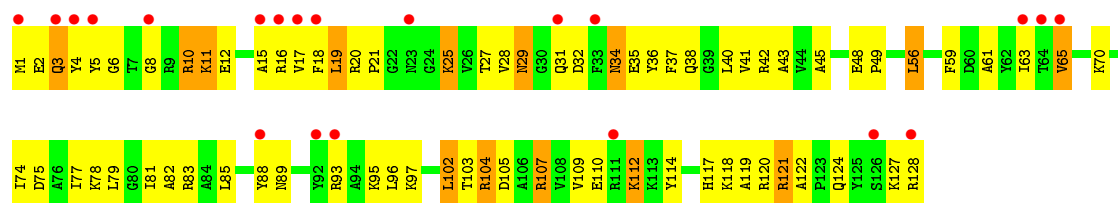


- Molecule 8: 30S ribosomal protein S8

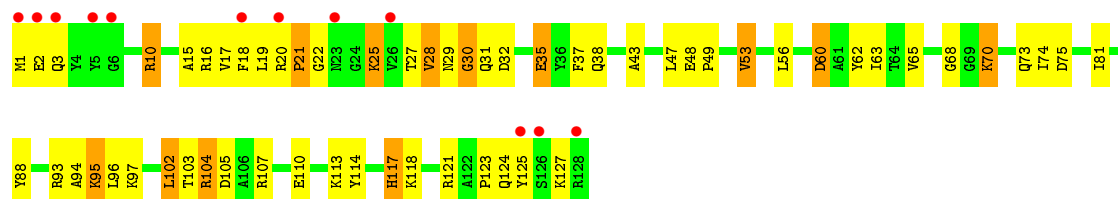


- Molecule 9: 30S ribosomal protein S9

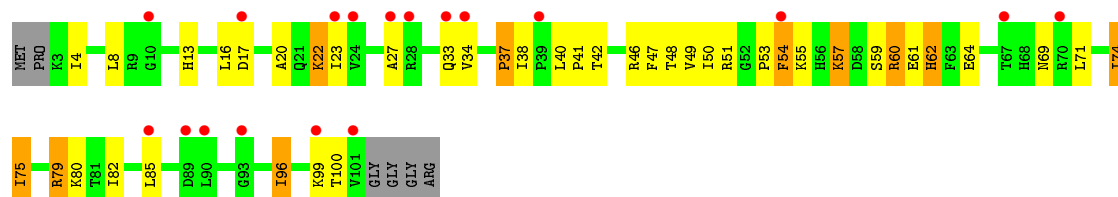




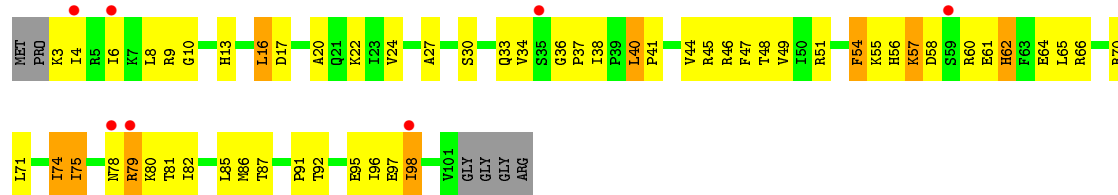
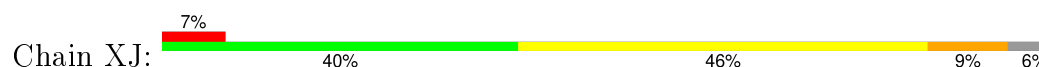
• Molecule 9: 30S ribosomal protein S9



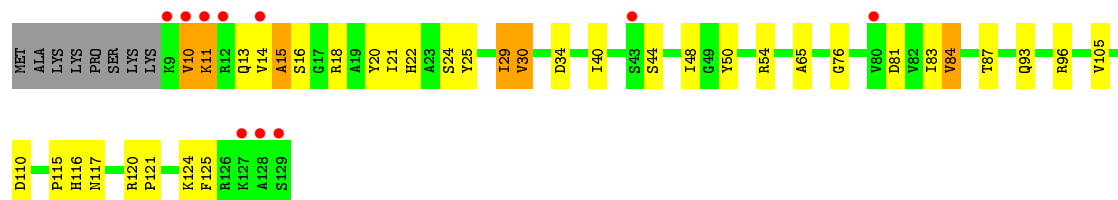
• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10

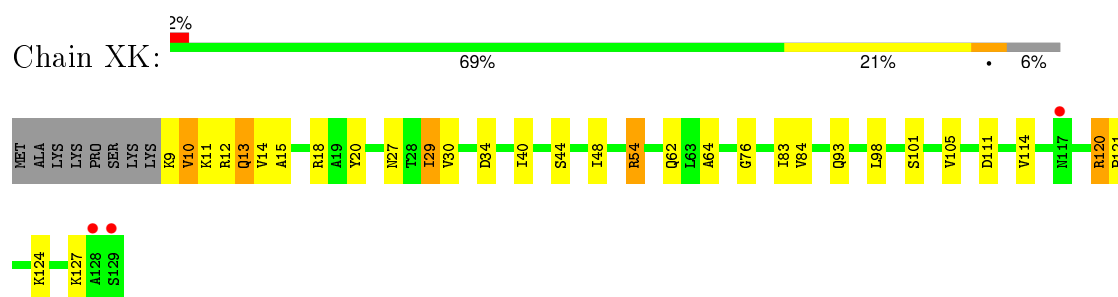


• Molecule 11: 30S ribosomal protein S11

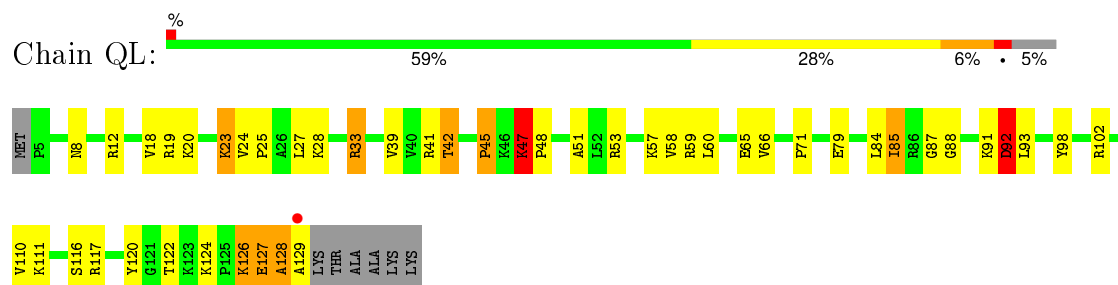


• Molecule 11: 30S ribosomal protein S11

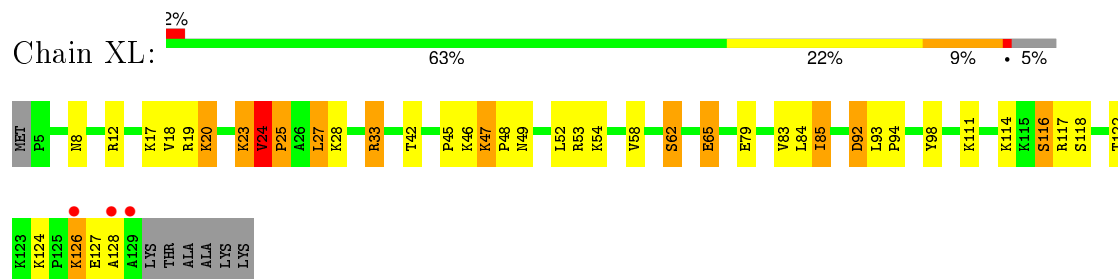




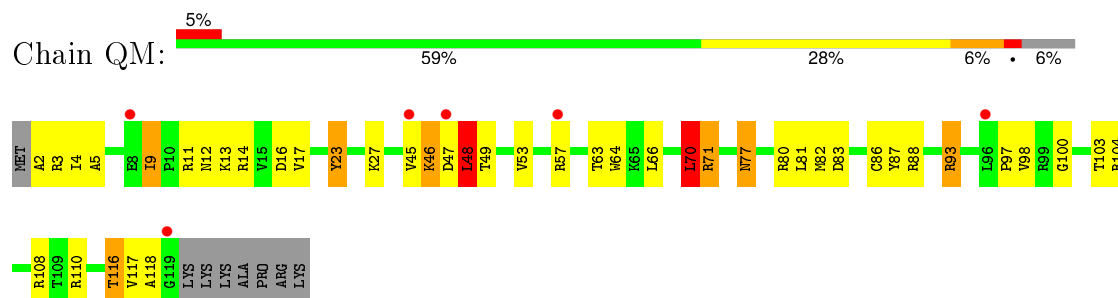
- Molecule 12: 30S ribosomal protein S12



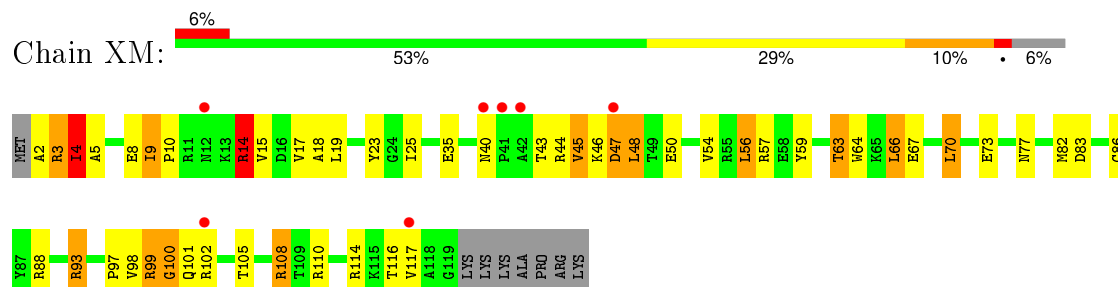
- Molecule 12: 30S ribosomal protein S12



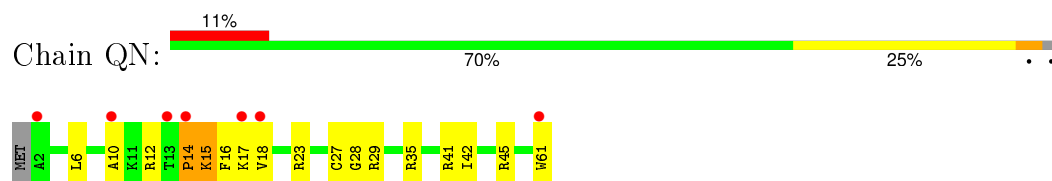
- Molecule 13: 30S ribosomal protein S13



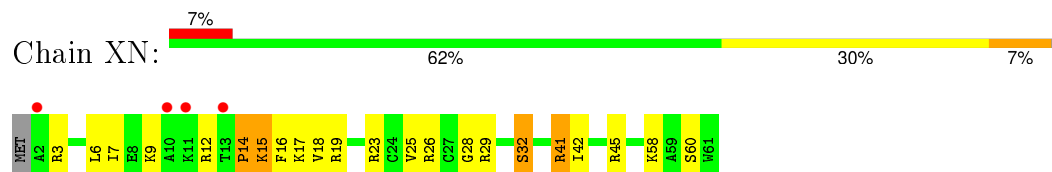
- Molecule 13: 30S ribosomal protein S13



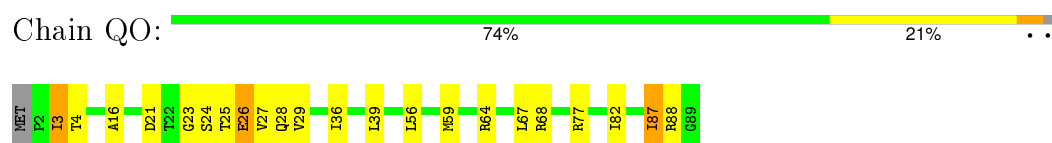
- Molecule 14: 30S ribosomal protein S14



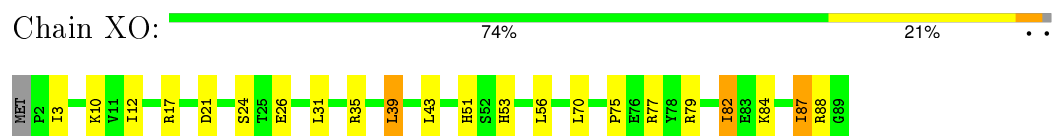
- Molecule 14: 30S ribosomal protein S14



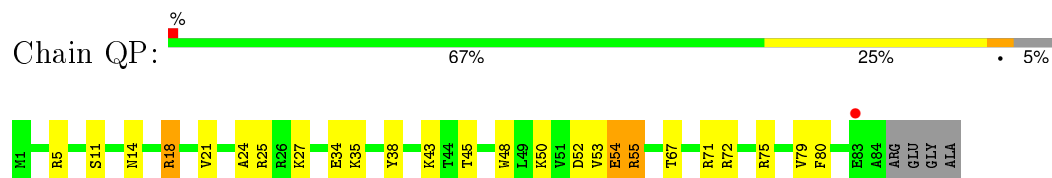
- Molecule 15: 30S ribosomal protein S15



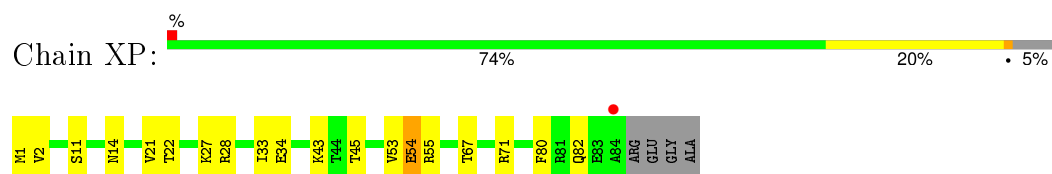
- Molecule 15: 30S ribosomal protein S15



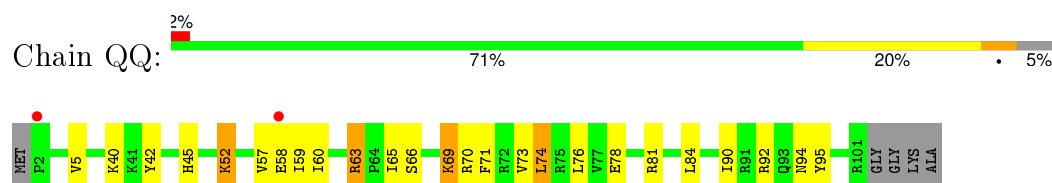
- Molecule 16: 30S ribosomal protein S16



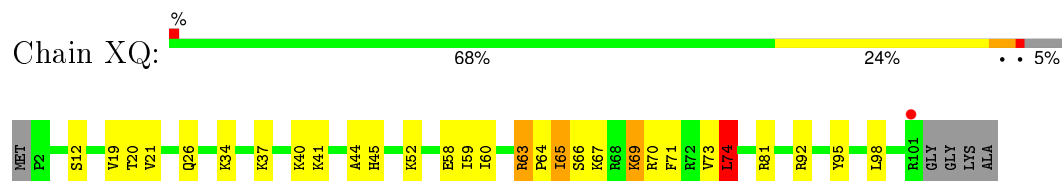
- Molecule 16: 30S ribosomal protein S16



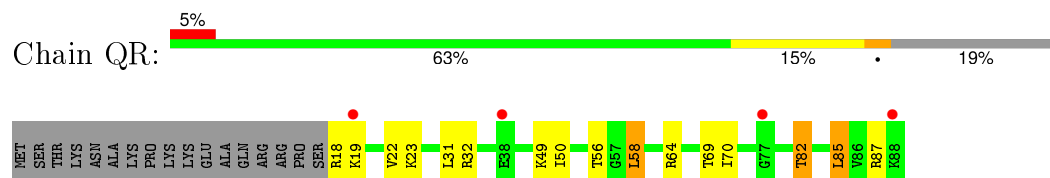
- Molecule 17: 30S ribosomal protein S17



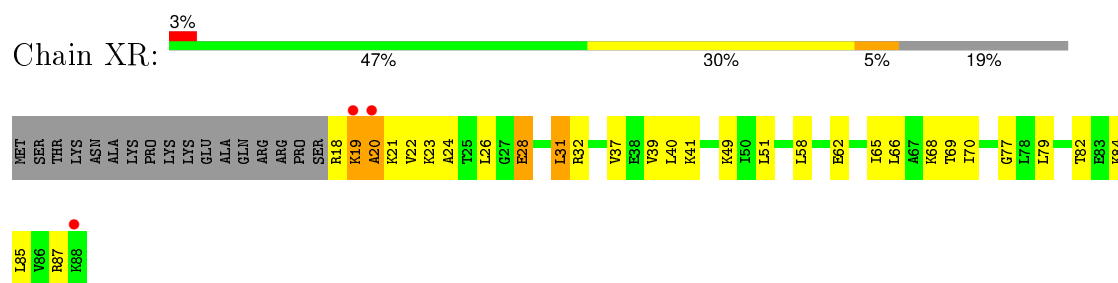
- Molecule 17: 30S ribosomal protein S17



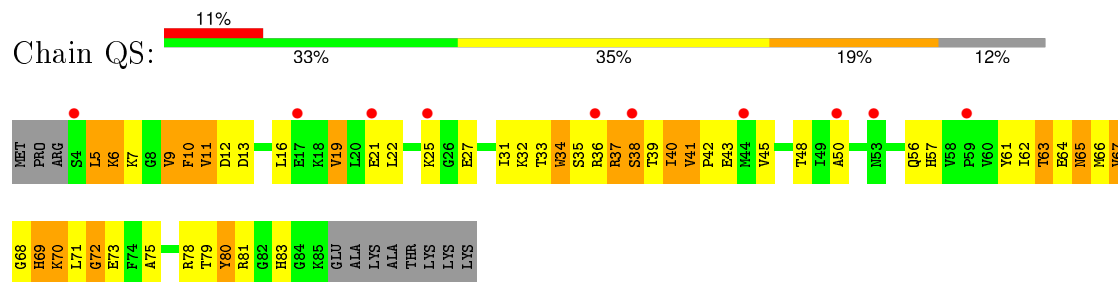
- Molecule 18: 30S ribosomal protein S18



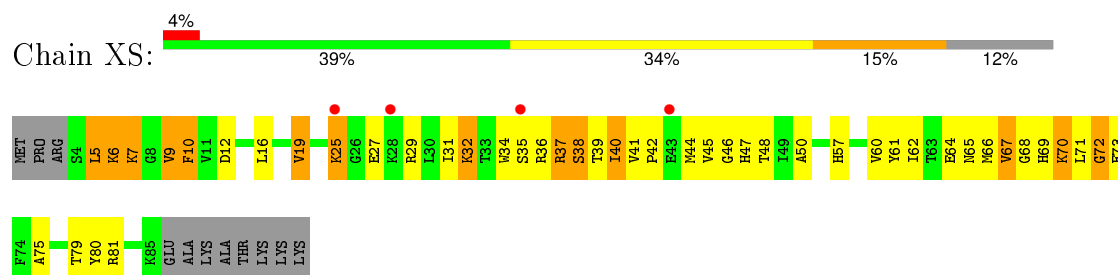
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

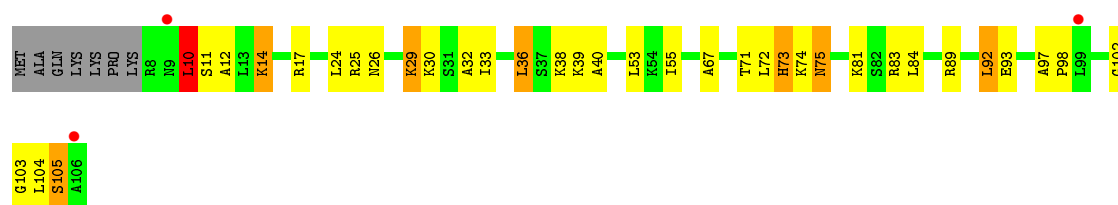


- Molecule 19: 30S ribosomal protein S19

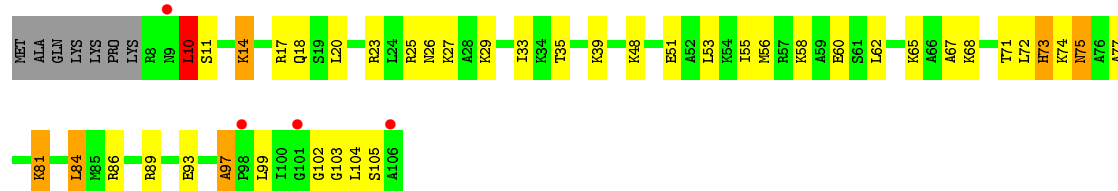


- Molecule 20: 30S ribosomal protein S20

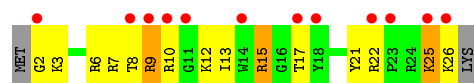
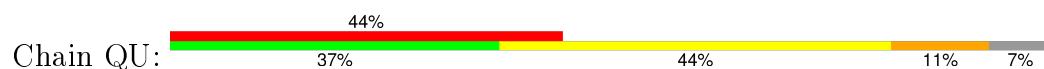




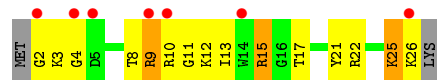
- Molecule 20: 30S ribosomal protein S20



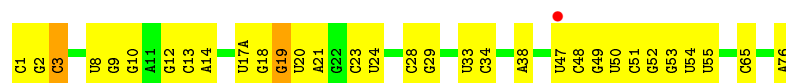
- Molecule 21: 30S ribosomal protein Thx



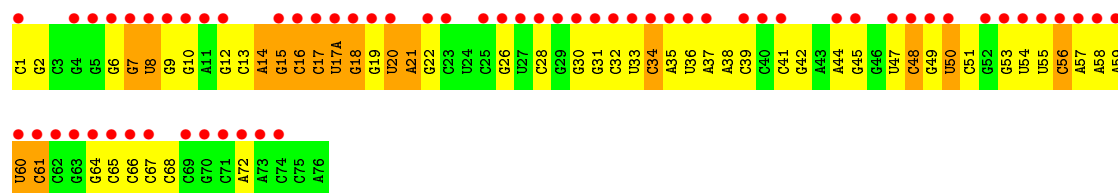
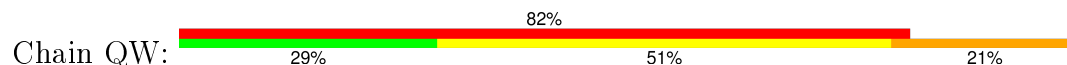
- Molecule 21: 30S ribosomal protein Thx



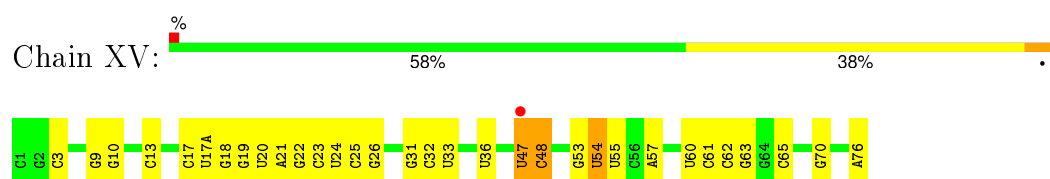
- Molecule 22: tRNA fMet



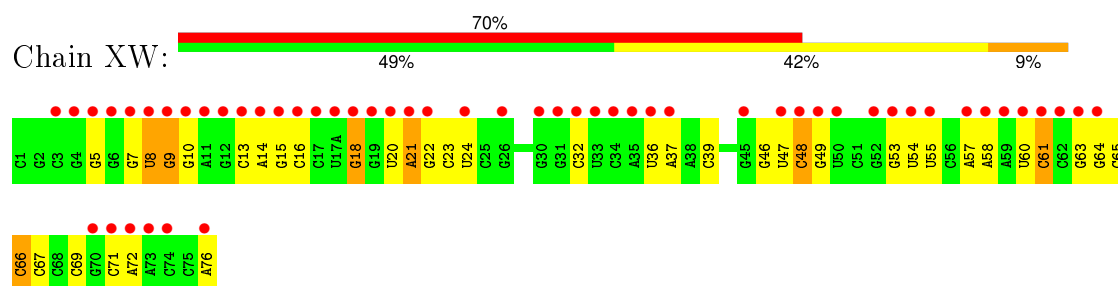
- Molecule 22: tRNA fMet



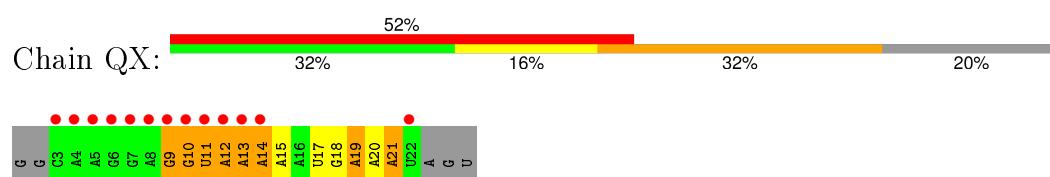
- Molecule 22: tRNA fMet



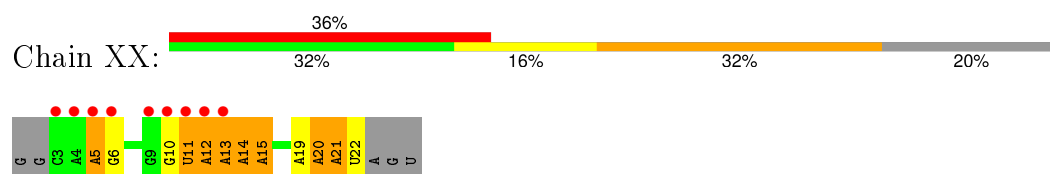
- Molecule 22: tRNA fMet



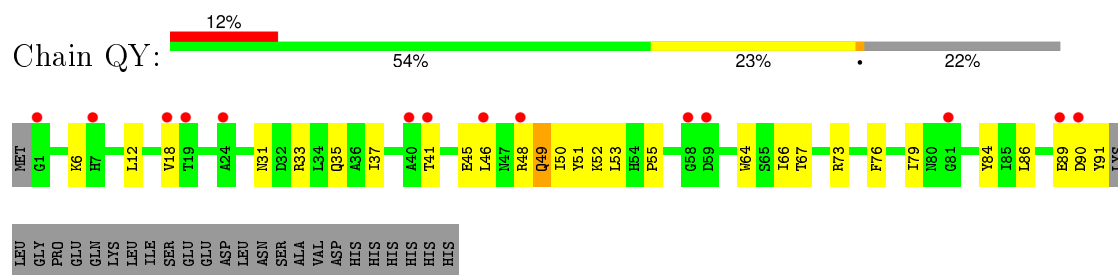
- Molecule 23: messenger RNA



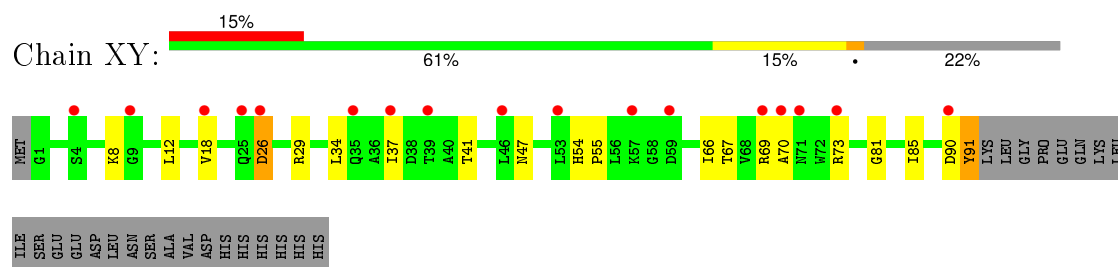
- Molecule 23: messenger RNA



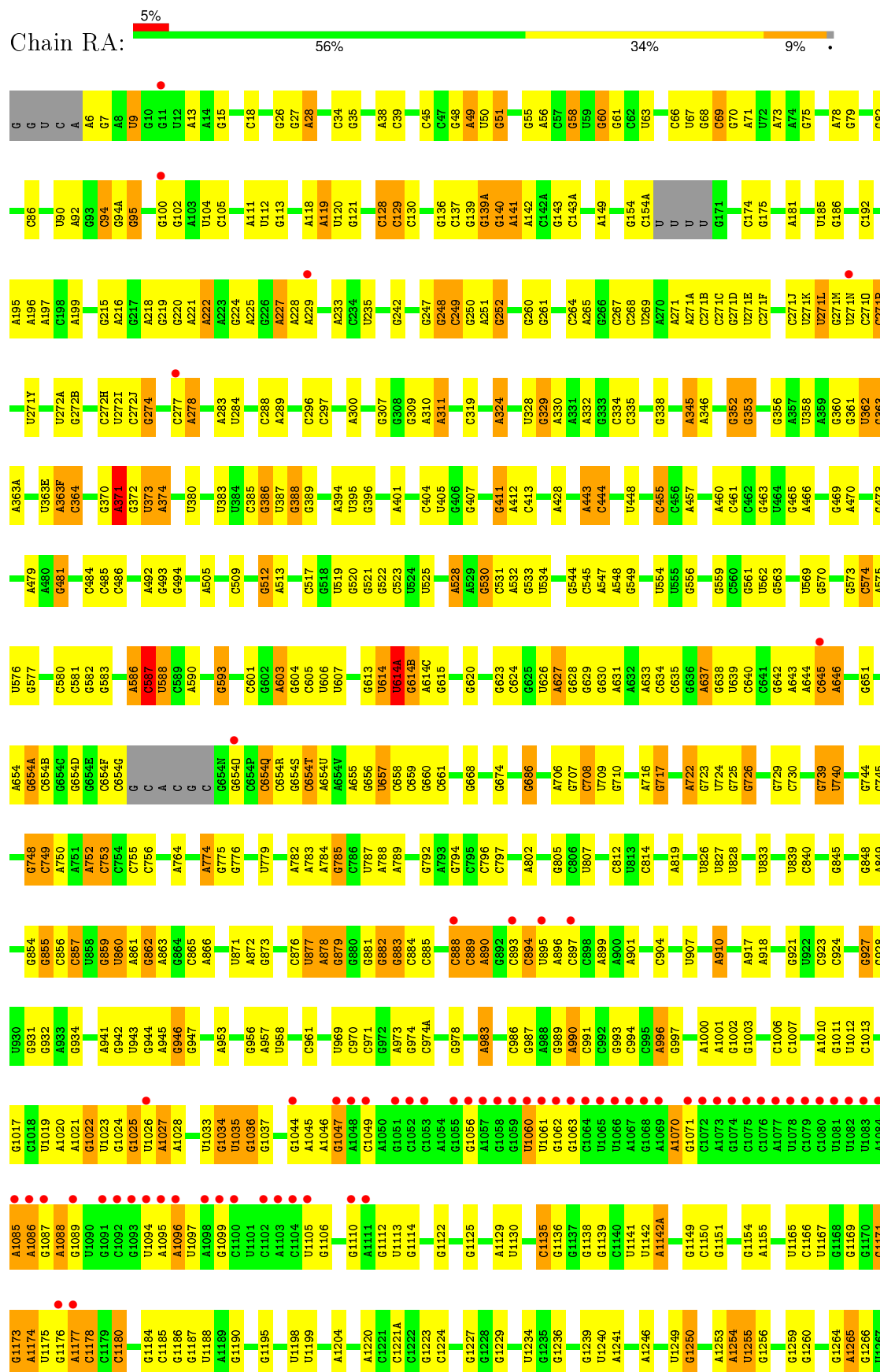
- Molecule 24: Host inhibition of growth B



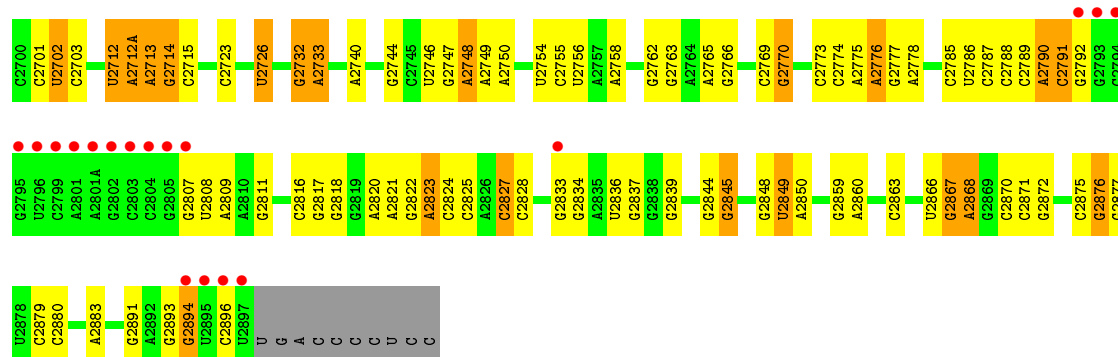
- Molecule 24: Host inhibition of growth B



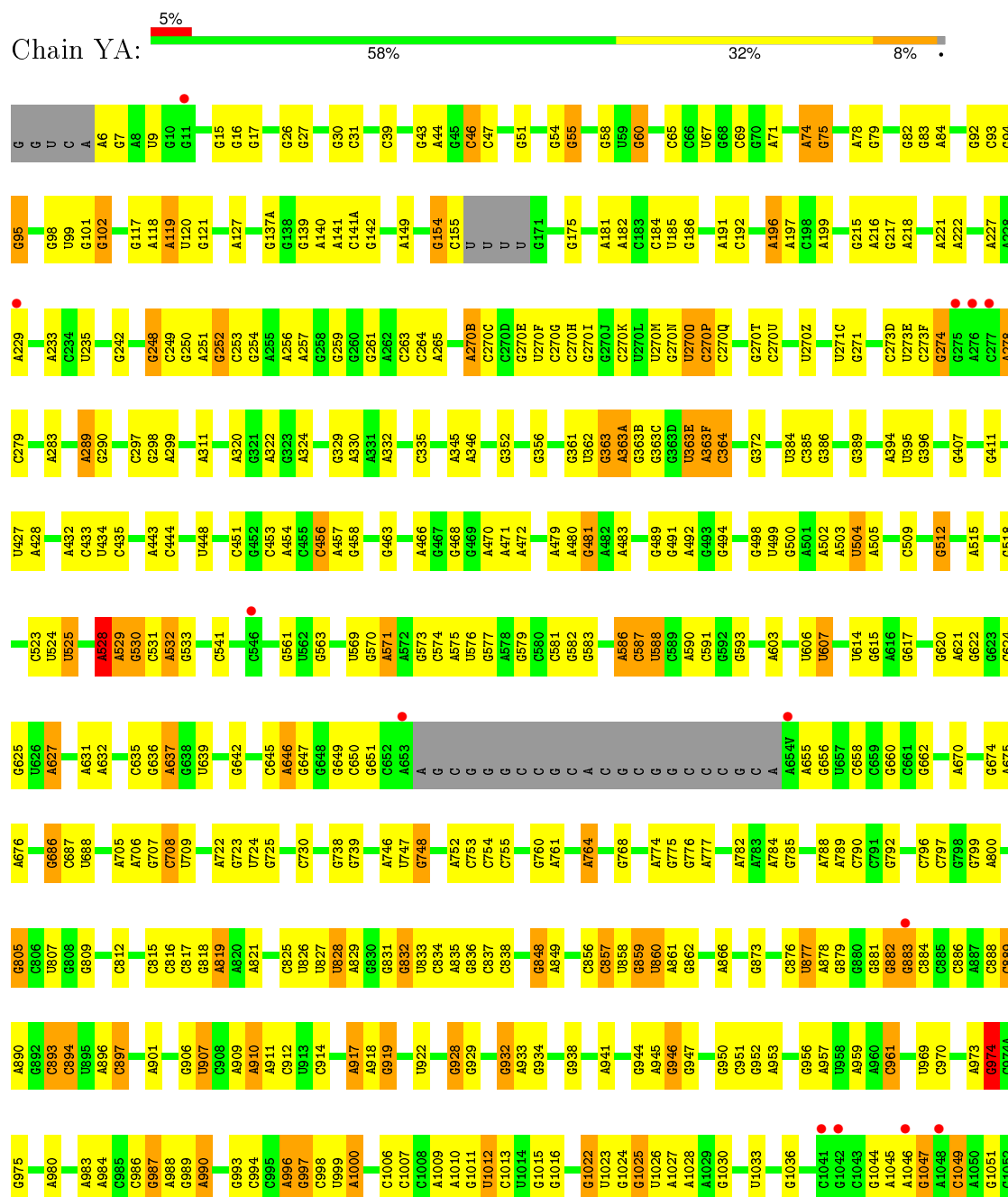
- Molecule 25: 23S rRNA



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

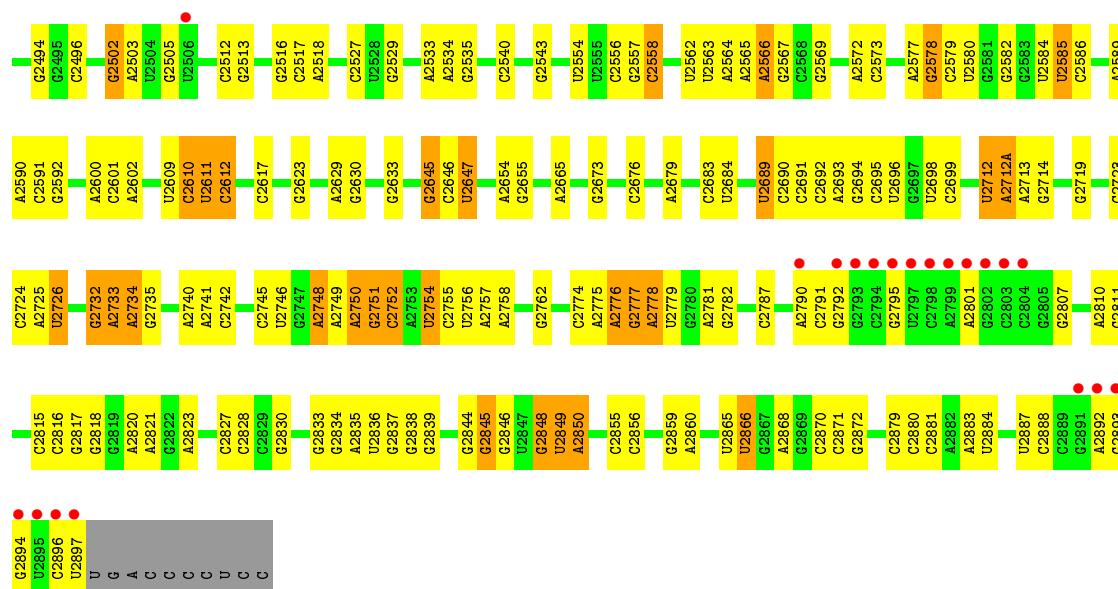


- Molecule 25: 23S rRNA

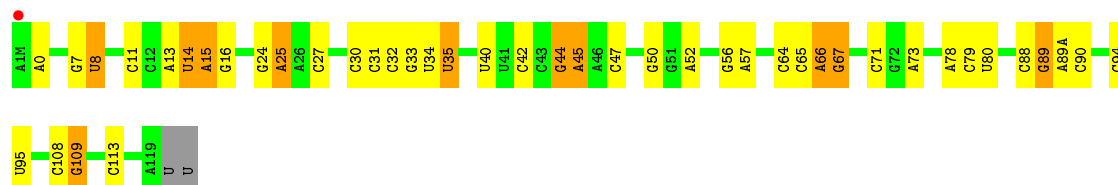




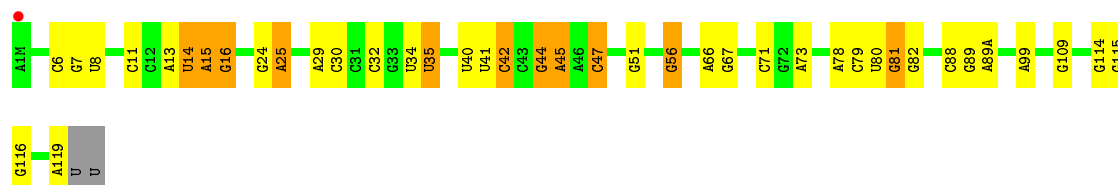
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G2410 | G2411 | G2307 | G2308 | A2309 | G2414 | G2415 | G2420 | G2421 | A2422 | U2423 | G2424 | A2425 | G2428 | G2429 | A2430 | A2434 | A2435 | U2438 | A2439 | G2440 | C2441 | C2442 | C2443 | G2444 | G2446 | G2447 | A2448 | U2449 | A2450 | G2458 | C2465 | G2466 | G2467 | G2468 | A2469 | G2472 | U2473 | C2474 | G2475 | A2476 | C2477 | A2478 | G2481 | C2482 | G2483 | C2484 | C2485 | A2493 | C2494 | G2495 | G2481 | G2482 | G2483 | U2401 | G2485 | C2402 | C2403 | G2404 | G2405 | A2406 | G2407 | A2305 | C2306 | G2130 | G2131 | U2132 | G2133 | A2134 | G2135 | C2136 | A2137 | C2138 | G2139 | C2140 | G2141 | C2142 | A2061 | A2062 | G2069 | G2070 | A2071 | U2074 | U2075 | G2080 | U2086 | G2087 | G2093 | U2099 | U2102 | C2103 | G2104 | C2105 | G2106 | C2107 | C2108 | U2109 | G2110 | C2111 | G2112 | U2113 | A2114 | G2115 | G2116 | A2117 | U2118 | A2119 | G2120 | G2121 | C2184 | C2185 | G2186 | U2188 | G2190 | G2191 | G2192 | C2193 | U2291 | C2292 | G2293 | C2294 | U2401 | G2402 | C2403 | C2404 | G2405 | U2406 | G2307 | G2308 | A2309 | U2208 | C2209 | G2210 | G2211 | A2212 | U2213 | G2215 | G2219 | G2224 | A2225 | C2226 | A2327 | G2328 | G2329 | A2336 | G2341 | C2342 | G2343 | U2344 | G2345 | A2346 | C2347 | G2356 | C2357 | G2365 | G2370 | G2371 | C2374 | G2381 | C2382 | G2383 | G2384 | C2385 | A2393 | C2394 | C2395 | G2396 | U2401 | G2402 | C2403 | C2404 | G2405 | U2406 | G2407 | A2408 | G2409 | G2410 | G2411 | G2412 | G2413 | G2414 | G2415 | G2416 | G2417 | G2418 | G2419 | G2420 | G2421 | G2422 | G2423 | G2424 | G2425 | G2426 | G2427 | G2428 | G2429 | G2430 | G2431 | G2432 | G2433 | G2434 | G2435 | G2436 | G2437 | G2438 | G2439 | G2440 | G2441 | G2442 | G2443 | G2444 | G2445 | G2446 | G2447 | G2448 | G2449 | G2450 | G2451 | G2452 | G2453 | G2454 | G2455 | G2456 | G2457 | G2458 | G2459 | G2460 | G2461 | G2462 | G2463 | G2464 | G2465 | G2466 | G2467 | G2468 | G2469 | G2470 | G2471 | G2472 | G2473 | G2474 | G2475 | G2476 | G2477 | G2478 | G2479 | G2480 | G2481 | G2482 | G2483 | G2484 | G2485 | G2486 | G2487 | G2488 | G2489 | G2490 | G2491 | G2492 | G2493 | G2494 | G2495 | G2496 | G2497 | G2498 | G2499 | G2500 | G2501 | G2502 | G2503 | G2504 | G2505 | G2506 | G2507 | G2508 | G2509 | G2510 | G2511 | G2512 | G2513 | G2514 | G2515 | G2516 | G2517 | G2518 | G2519 | G2520 | G2521 | G2522 | G2523 | G2524 | G2525 | G2526 | G2527 | G2528 | G2529 | G2530 | G2531 | G2532 | G2533 | G2534 | G2535 | G2536 | G2537 | G2538 | G2539 | G2540 | G2541 | G2542 | G2543 | G2544 | G2545 | G2546 | G2547 | G2548 | G2549 | G2550 | G2551 | G2552 | G2553 | G2554 | G2555 | G2556 | G2557 | G2558 | G2559 | G2560 | G2561 | G2562 | G2563 | G2564 | G2565 | G2566 | G2567 | G2568 | G2569 | G2570 | G2571 | G2572 | G2573 | G2574 | G2575 | G2576 | G2577 | G2578 | G2579 | G2580 | G2581 | G2582 | G2583 | G2584 | G2585 | G2586 | G2587 | G2588 | G2589 | G2590 | G2591 | G2592 | G2593 | G2594 | G2595 | G2596 | G2597 | G2598 | G2599 | G2600 | G2601 | G2602 | G2603 | G2604 | G2605 | G2606 | G2607 | G2608 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| G3109 | G3110 | G3111 | G3112 | G3113 | G3114 | G3115 | G3116 | G3117 | G3118 | G3119 | G3120 | G3121 | G3122 | G3123 | G3124 | G3125 | G3126 | G3127 | G3128 | G3129 | G3130 | G3131 | G3132 | G3133 | G3134 | G3135 | G3136 | G3137 | G3138 | G3139 | G3140 | G3141 | G3142 | G3143 | G3144 | G3145 | G3146 | G3147 | G3148 | G3149 | G3150 | G3151 | G3152 | G3153 | G3154 | G3155 | G3156 | G3157 | G3158 | G3159 | G3160 | G3161 | G3162 | G3163 | G3164 | G3165 | G3166 | G3167 | G3168 | G3169 | G3170 | G3171 | G3172 | G3173 | G3174 | G3175 | G3176 | G3177 | G3178 | G3179 | G3180 | G3181 | G3182 | G3183 | G3184 | G3185 | G3186 | G3187 | G3188 | G3189 | G3190 | G3191 | G3192 | G3193 | G3194 | G3195 | G3196 | G3197 | G3198 | G3199 | G3200 | G3201 | G3202 | G3203 | G3204 | G3205 | G3206 | G3207 | G3208 | G3209 | G3210 | G3211 | G3212 | G3213 | G3214 | G3215 | G3216 | G3217 | G3218 | G3219 | G3220 | G3221 | G3222 | G3223 | G3224 | G3225 | G3226 | G3227 | G3228 | G3229 | G3230 | G3231 | G3232 | G3233 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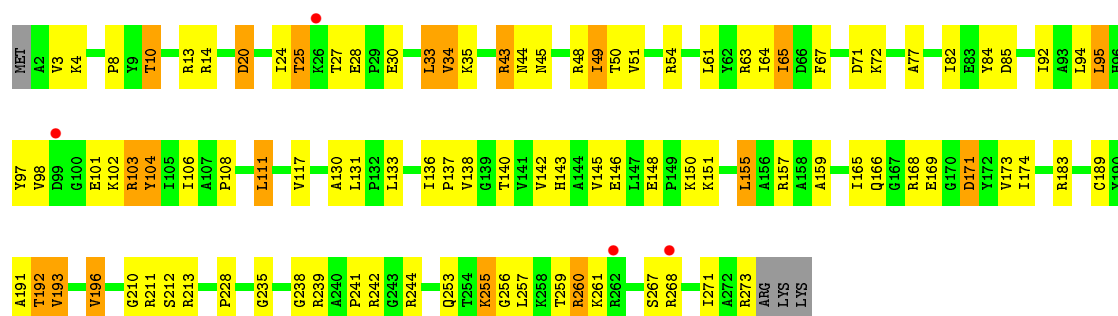
- Molecule 26: 5S rRNA



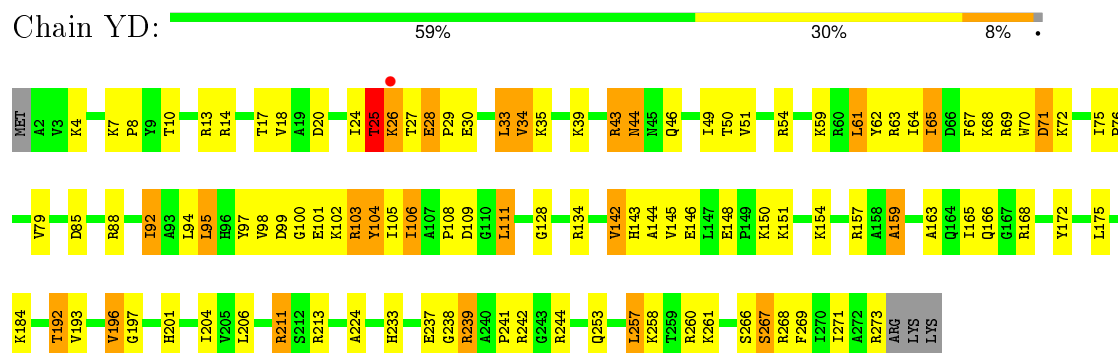
- Molecule 26: 5S rRNA



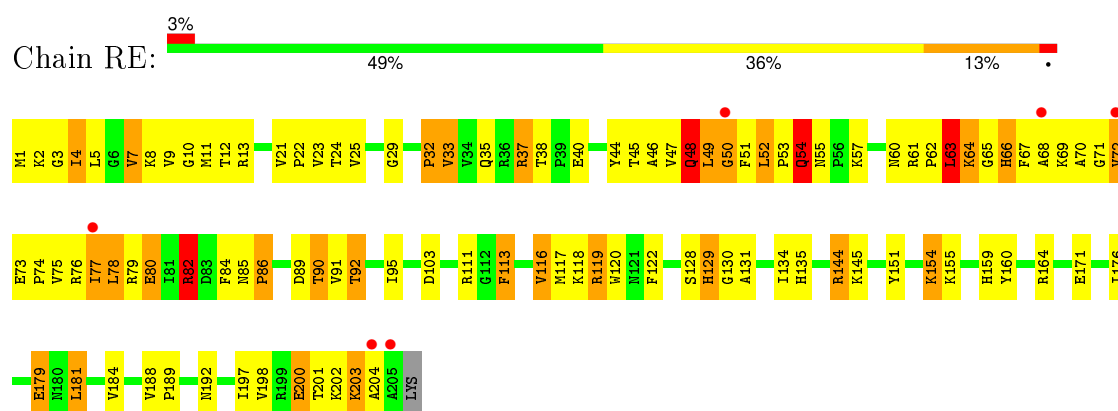
- Molecule 27: 50S ribosomal protein L2



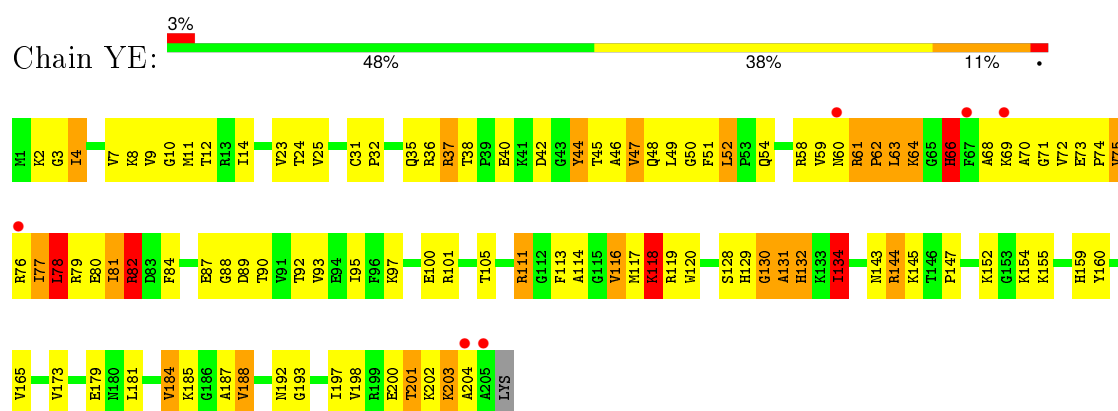
- Molecule 27: 50S ribosomal protein L2



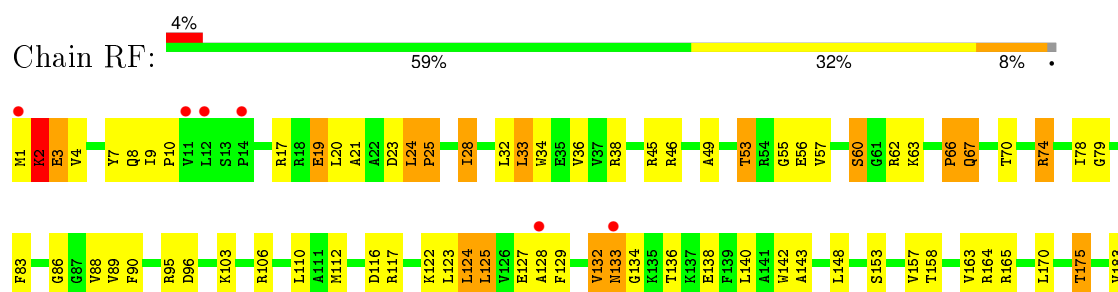
- Molecule 28: 50S ribosomal protein L3

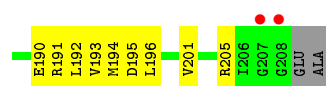


- Molecule 28: 50S ribosomal protein L3

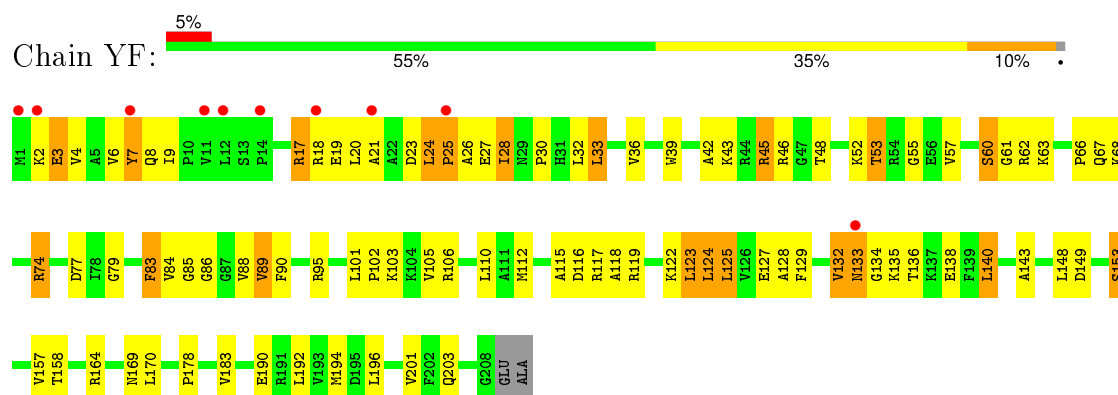


- Molecule 29: 50S ribosomal protein L4

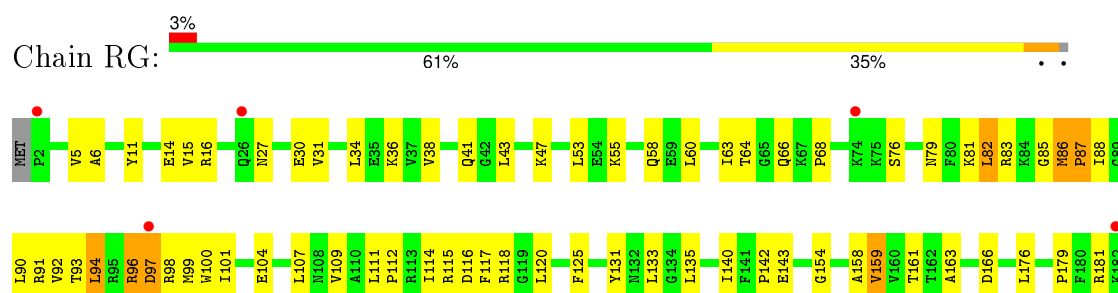




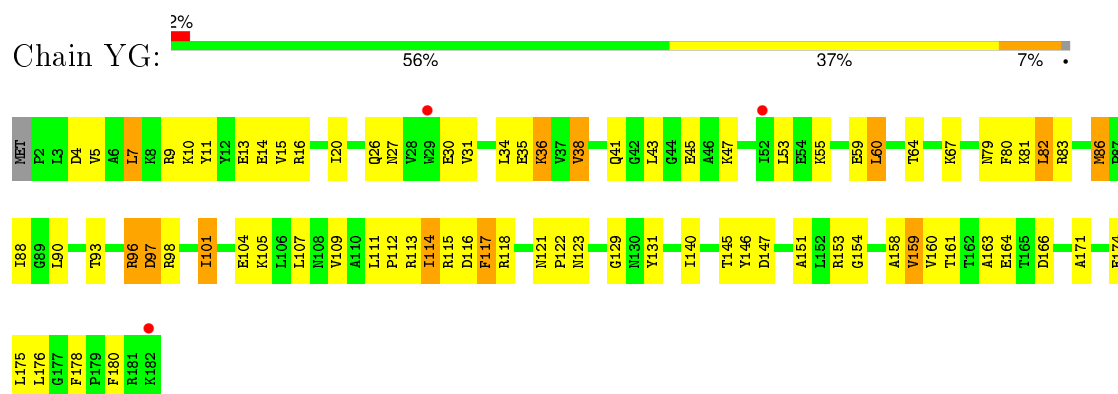
- Molecule 29: 50S ribosomal protein L4



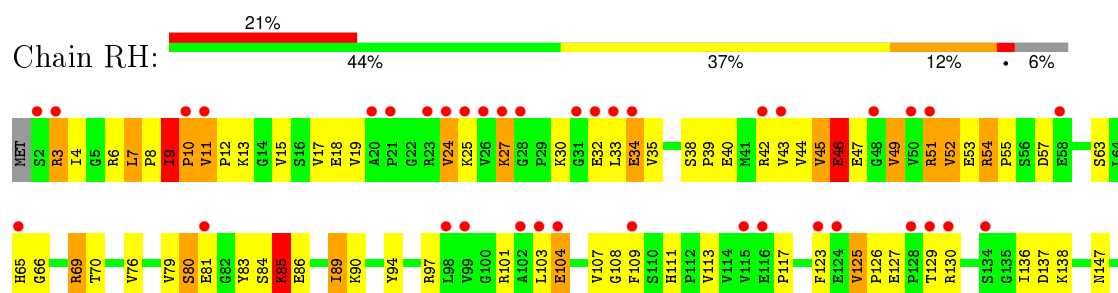
- Molecule 30: 50S ribosomal protein L5



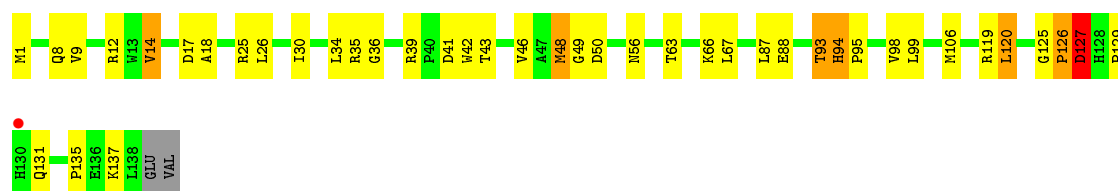
- Molecule 30: 50S ribosomal protein L5



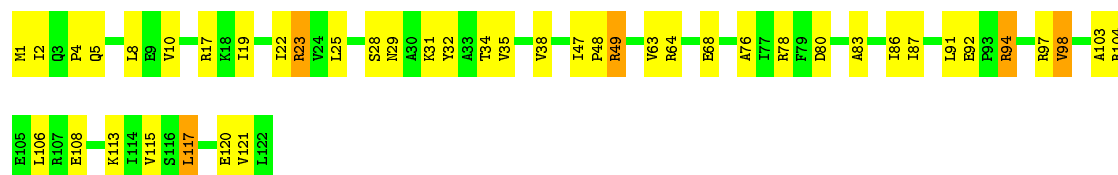
- Molecule 31: 50S ribosomal protein L6



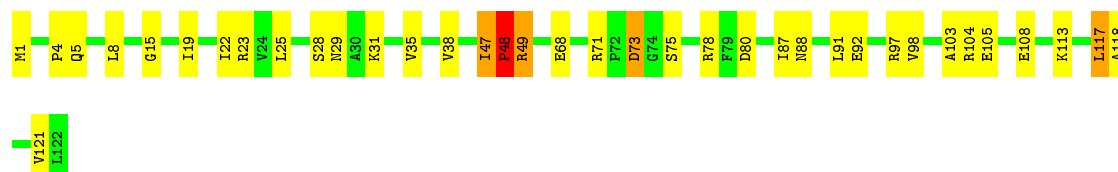




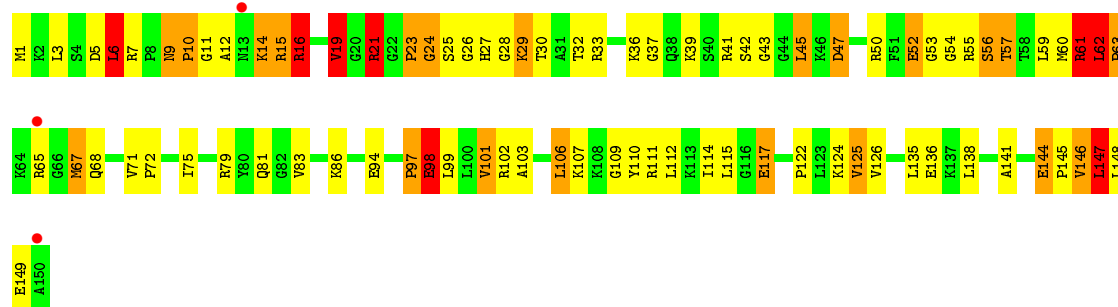
- Molecule 34: 50S ribosomal protein L14



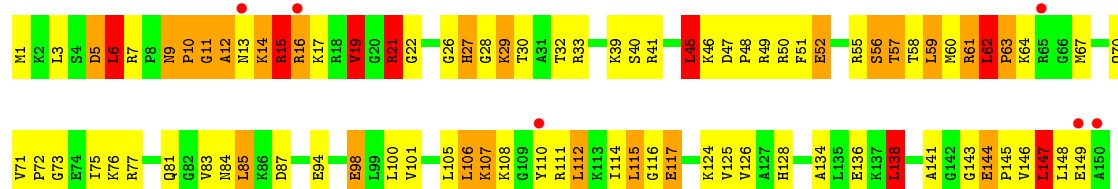
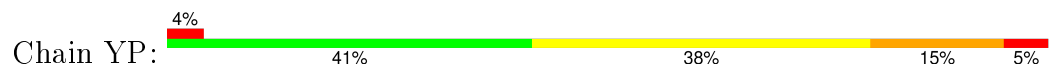
- Molecule 34: 50S ribosomal protein L14



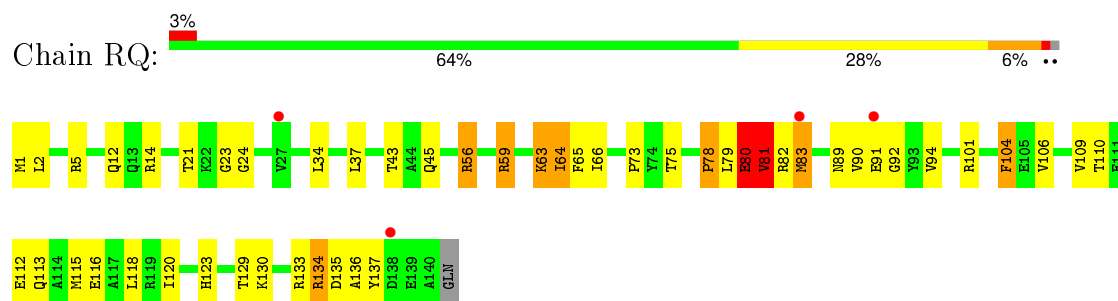
- Molecule 35: 50S ribosomal protein L15



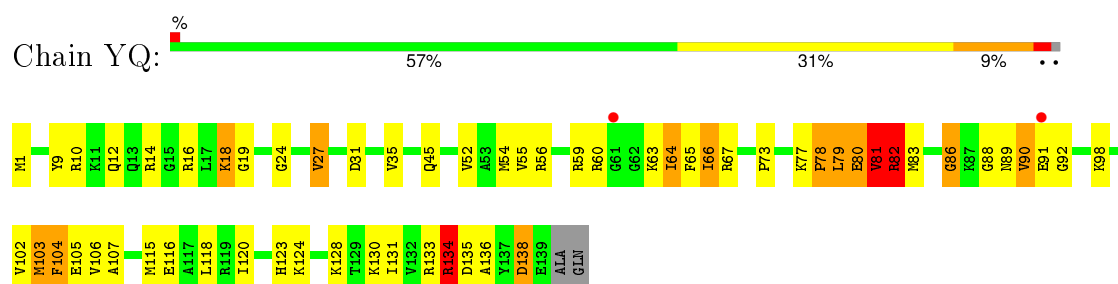
- Molecule 35: 50S ribosomal protein L15



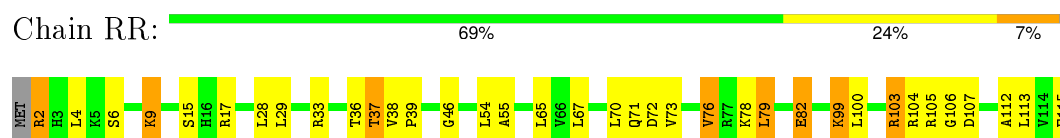
- Molecule 36: 50S ribosomal protein L16



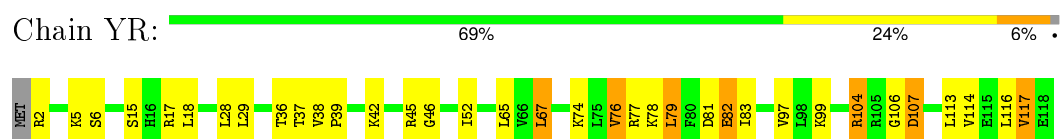
- Molecule 36: 50S ribosomal protein L16



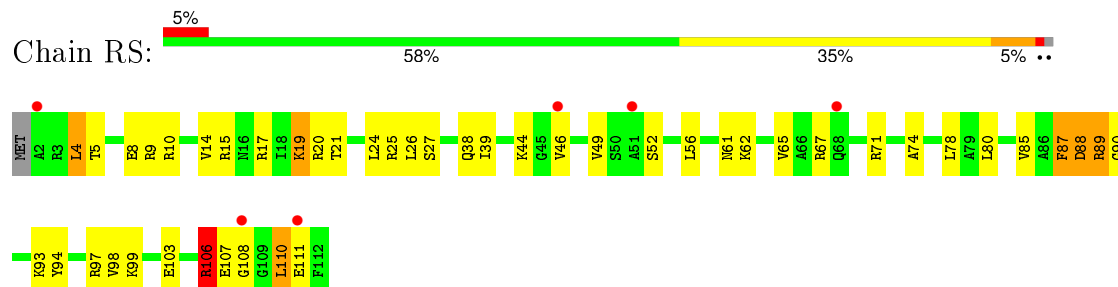
- Molecule 37: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L17

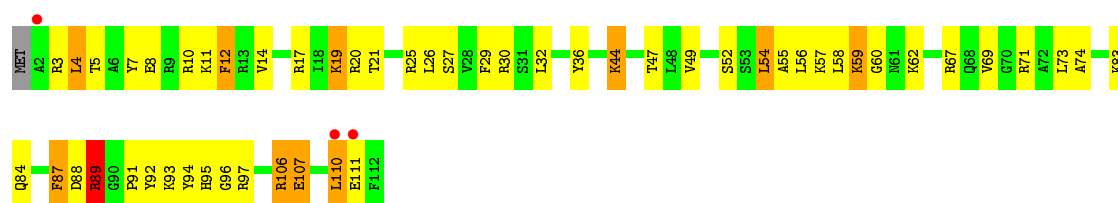


- Molecule 38: 50S ribosomal protein L18

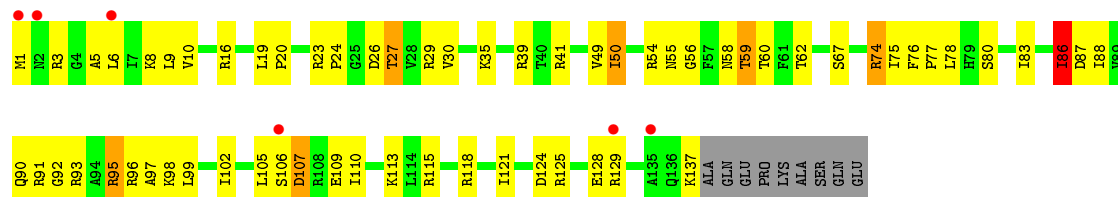


- Molecule 38: 50S ribosomal protein L18

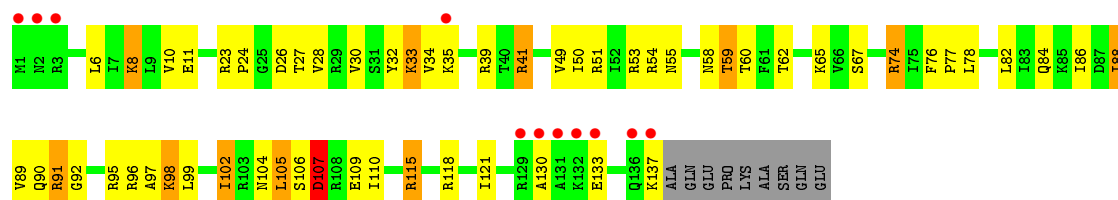




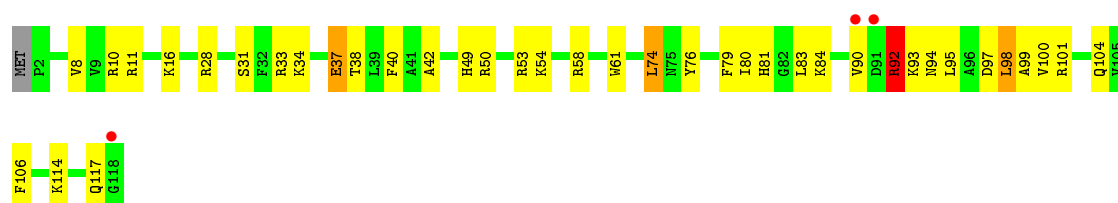
- Molecule 39: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L20



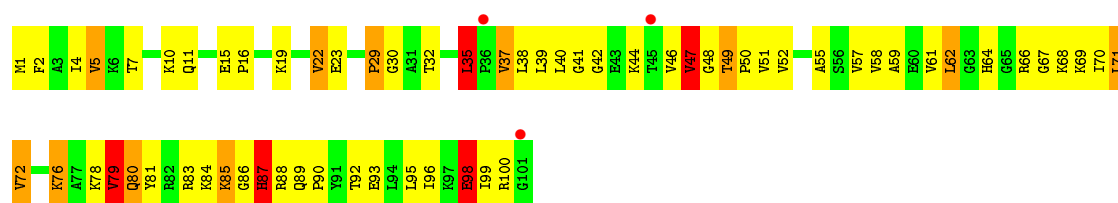
- Molecule 40: 50S ribosomal protein L20



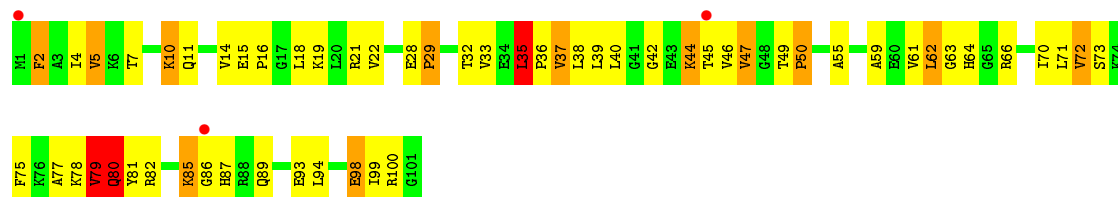
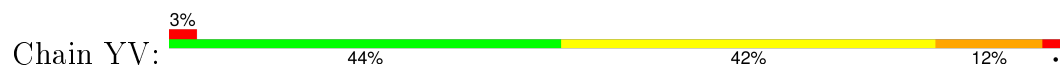
- Molecule 41: 50S ribosomal protein L21



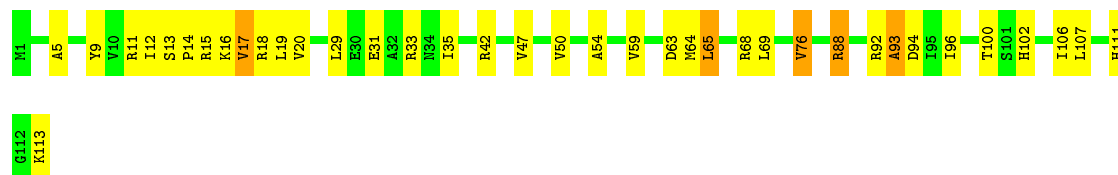




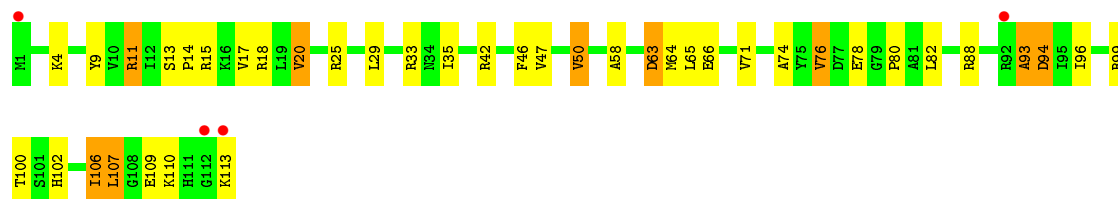
• Molecule 41: 50S ribosomal protein L21



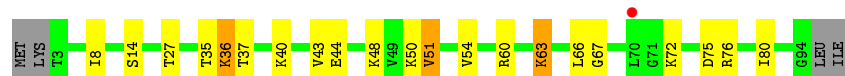
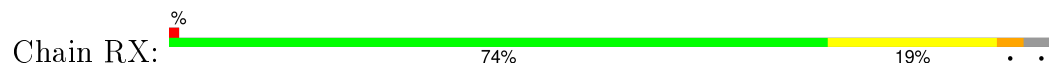
• Molecule 42: 50S ribosomal protein L22



• Molecule 42: 50S ribosomal protein L22

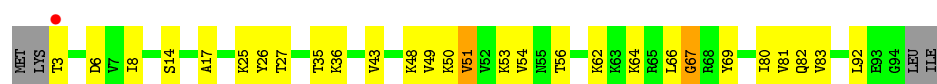


• Molecule 43: 50S ribosomal protein L23

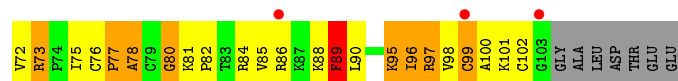


• Molecule 43: 50S ribosomal protein L23

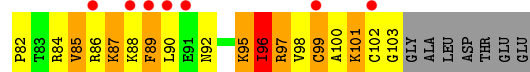
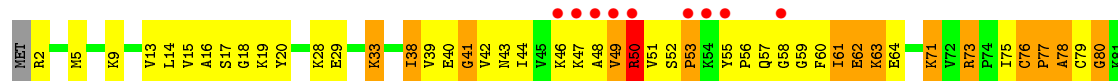




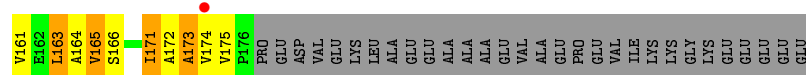
- Molecule 44: 50S ribosomal protein L24



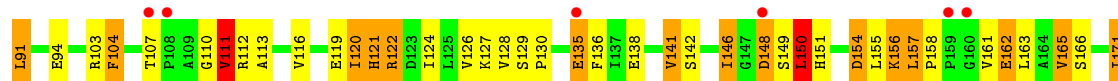
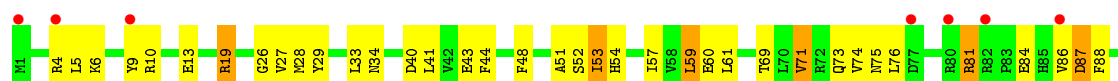
- Molecule 44: 50S ribosomal protein L24

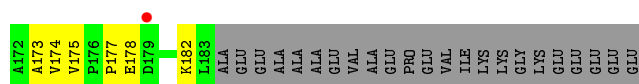


- Molecule 45: 50S ribosomal protein L25

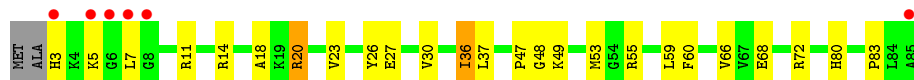


- Molecule 45: 50S ribosomal protein L25





- Molecule 46: 50S ribosomal protein L27



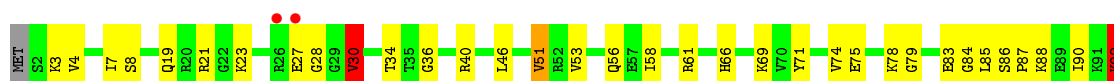
- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L28

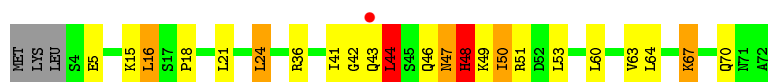


- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29





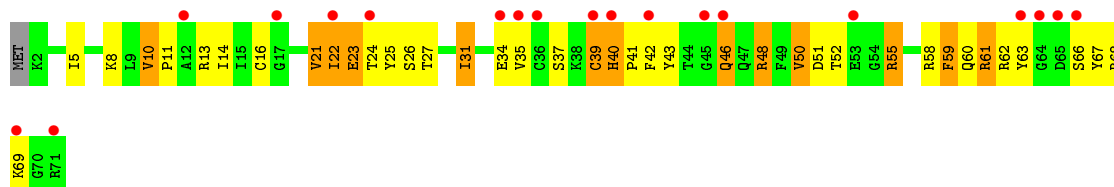
- Molecule 49: 50S ribosomal protein L30



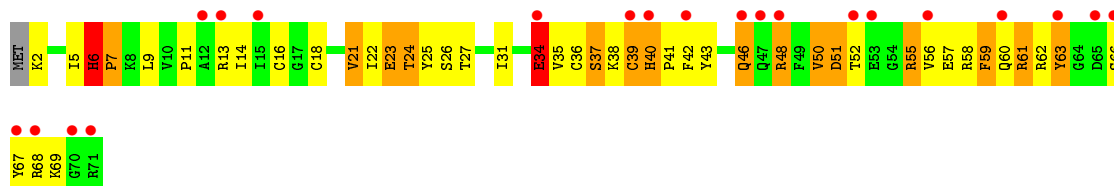
- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31

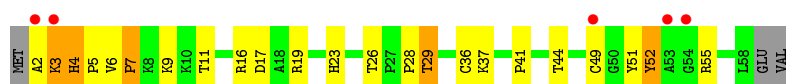


- Molecule 51: 50S ribosomal protein L32

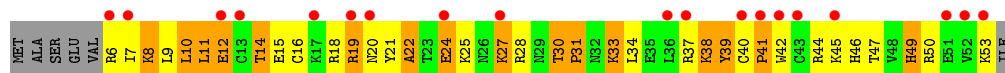
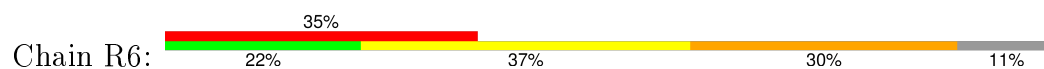


- Molecule 51: 50S ribosomal protein L32

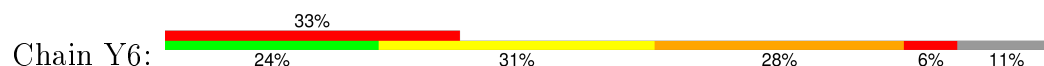




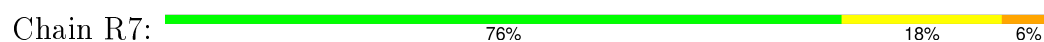
- Molecule 52: 50S ribosomal protein L33



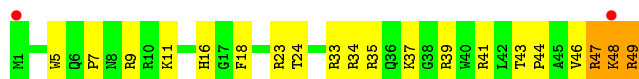
- Molecule 52: 50S ribosomal protein L33



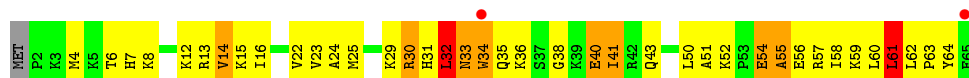
- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35

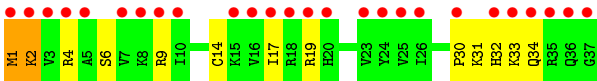


- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36





● Molecule 55: 50S ribosomal protein L36



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 214.11Å 453.88Å 607.59Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 34.93 – 3.40<br>34.99 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (34.93-3.40)<br>98.9 (34.99-3.20)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.21  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.55 (at 3.18Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.8.2_1309)                          | Depositor        |
| R, $R_{free}$   | 0.202 , 0.234<br>0.216 , 0.249                              | Depositor<br>DCC |
| $R_{free}$ test set   | 36504 reflections (4.82%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 72.8  | Xtriage          |
| Anisotropy  | 0.176   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 76.8   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Outliers  | 0 of 951681 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 297549  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 91.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, A2M

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$     |
| 1   | QA    | 0.30         | 1/36346 (0.0%) | 0.79        | 15/56724 (0.0%) |
| 1   | XA    | 0.31         | 0/36276        | 0.80        | 19/56615 (0.0%) |
| 2   | QB    | 0.25         | 0/1950         | 0.49        | 0/2630          |
| 2   | XB    | 0.26         | 0/1950         | 0.49        | 1/2630 (0.0%)   |
| 3   | QC    | 0.24         | 0/1636         | 0.47        | 0/2205          |
| 3   | XC    | 0.27         | 0/1636         | 0.48        | 0/2205          |
| 4   | QD    | 0.28         | 0/1733         | 0.50        | 0/2318          |
| 4   | XD    | 0.28         | 0/1733         | 0.50        | 0/2318          |
| 5   | QE    | 0.28         | 0/1195         | 0.48        | 0/1609          |
| 5   | XE    | 0.29         | 0/1195         | 0.48        | 0/1609          |
| 6   | QF    | 0.25         | 0/856          | 0.45        | 0/1154          |
| 6   | XF    | 0.28         | 0/856          | 0.45        | 0/1154          |
| 7   | QG    | 0.24         | 0/1276         | 0.45        | 0/1709          |
| 7   | XG    | 0.26         | 0/1276         | 0.45        | 0/1709          |
| 8   | QH    | 0.25         | 0/1136         | 0.47        | 0/1527          |
| 8   | XH    | 0.27         | 0/1136         | 0.45        | 0/1527          |
| 9   | QI    | 0.25         | 0/1037         | 0.48        | 0/1389          |
| 9   | XI    | 0.26         | 0/1037         | 0.48        | 0/1389          |
| 10  | QJ    | 0.24         | 0/814          | 0.45        | 0/1095          |
| 10  | XJ    | 0.24         | 0/814          | 0.46        | 0/1095          |
| 11  | QK    | 0.27         | 0/916          | 0.44        | 0/1234          |
| 11  | XK    | 0.28         | 0/916          | 0.48        | 0/1234          |
| 12  | QL    | 0.31         | 0/991          | 0.52        | 1/1327 (0.1%)   |
| 12  | XL    | 0.36         | 1/991 (0.1%)   | 0.56        | 1/1327 (0.1%)   |
| 13  | QM    | 0.26         | 0/947          | 0.53        | 1/1270 (0.1%)   |
| 13  | XM    | 0.25         | 0/947          | 0.52        | 0/1270          |
| 14  | QN    | 0.25         | 0/501          | 0.47        | 0/664           |
| 14  | XN    | 0.29         | 0/501          | 0.49        | 0/664           |
| 15  | QO    | 0.24         | 0/745          | 0.39        | 0/992           |
| 15  | XO    | 0.27         | 0/745          | 0.43        | 0/992           |
| 16  | QP    | 0.27         | 0/721          | 0.46        | 0/970           |
| 16  | XP    | 0.25         | 0/721          | 0.45        | 0/970           |



| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 17  | QQ    | 0.26         | 0/847          | 0.46        | 0/1131           |
| 17  | XQ    | 0.30         | 0/847          | 0.47        | 0/1131           |
| 18  | QR    | 0.25         | 0/590          | 0.48        | 0/782            |
| 18  | XR    | 0.27         | 0/590          | 0.51        | 0/782            |
| 19  | QS    | 0.27         | 0/670          | 0.53        | 0/901            |
| 19  | XS    | 0.29         | 0/670          | 0.52        | 0/901            |
| 20  | QT    | 0.25         | 0/765          | 0.49        | 1/1007 (0.1%)    |
| 20  | XT    | 0.25         | 0/765          | 0.48        | 0/1007           |
| 21  | QU    | 0.23         | 0/221          | 0.46        | 0/288            |
| 21  | XU    | 0.25         | 0/221          | 0.44        | 0/288            |
| 22  | QV    | 0.28         | 0/1832         | 0.77        | 0/2855           |
| 22  | QW    | 0.20         | 0/1832         | 0.75        | 0/2855           |
| 22  | XV    | 0.31         | 0/1832         | 0.80        | 0/2855           |
| 22  | XW    | 0.19         | 0/1832         | 0.77        | 0/2855           |
| 23  | QX    | 0.44         | 0/417          | 0.87        | 0/649            |
| 23  | XX    | 0.43         | 0/417          | 0.96        | 0/649            |
| 24  | QY    | 0.31         | 0/762          | 0.45        | 0/1028           |
| 24  | XY    | 0.26         | 0/762          | 0.42        | 0/1028           |
| 25  | RA    | 0.39         | 4/69742 (0.0%) | 0.85        | 22/108874 (0.0%) |
| 25  | YA    | 0.39         | 1/69356 (0.0%) | 0.86        | 21/108271 (0.0%) |
| 26  | RB    | 0.28         | 0/2928         | 0.79        | 0/4568           |
| 26  | YB    | 0.30         | 0/2928         | 0.80        | 0/4568           |
| 27  | RD    | 0.34         | 0/2165         | 0.56        | 0/2919           |
| 27  | YD    | 0.37         | 0/2165         | 0.60        | 0/2919           |
| 28  | RE    | 0.33         | 0/1601         | 0.58        | 0/2160           |
| 28  | YE    | 0.33         | 0/1601         | 0.58        | 0/2160           |
| 29  | RF    | 0.35         | 0/1662         | 0.58        | 0/2249           |
| 29  | YF    | 0.31         | 0/1662         | 0.58        | 0/2249           |
| 30  | RG    | 0.25         | 0/1499         | 0.46        | 0/2016           |
| 30  | YG    | 0.25         | 0/1499         | 0.46        | 0/2016           |
| 31  | RH    | 0.25         | 0/1332         | 0.60        | 1/1802 (0.1%)    |
| 31  | YH    | 0.29         | 0/1332         | 0.67        | 1/1802 (0.1%)    |
| 32  | RI    | 0.24         | 0/1151         | 0.54        | 0/1558           |
| 32  | YI    | 0.28         | 0/1151         | 0.58        | 0/1558           |
| 33  | RN    | 0.28         | 0/1131         | 0.50        | 0/1525           |
| 33  | YN    | 0.29         | 0/1131         | 0.51        | 0/1525           |
| 34  | RO    | 0.32         | 0/943          | 0.51        | 0/1269           |
| 34  | YO    | 0.33         | 0/943          | 0.53        | 0/1269           |
| 35  | RP    | 0.34         | 0/1162         | 0.66        | 0/1544           |
| 35  | YP    | 0.35         | 0/1162         | 0.70        | 2/1544 (0.1%)    |
| 36  | RQ    | 0.34         | 0/1133         | 0.57        | 0/1515           |
| 36  | YQ    | 0.35         | 0/1128         | 0.58        | 1/1508 (0.1%)    |
| 37  | RR    | 0.27         | 0/974          | 0.51        | 0/1302           |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 37  | YR    | 0.30         | 0/974           | 0.53        | 0/1302           |
| 38  | RS    | 0.25         | 0/892           | 0.48        | 0/1187           |
| 38  | YS    | 0.29         | 0/892           | 0.54        | 0/1187           |
| 39  | RT    | 0.27         | 0/1155          | 0.46        | 0/1542           |
| 39  | YT    | 0.30         | 0/1155          | 0.47        | 0/1542           |
| 40  | RU    | 0.32         | 0/982           | 0.53        | 0/1306           |
| 40  | YU    | 0.33         | 0/982           | 0.52        | 0/1306           |
| 41  | RV    | 0.37         | 0/790           | 0.69        | 1/1057 (0.1%)    |
| 41  | YV    | 0.35         | 0/790           | 0.68        | 1/1057 (0.1%)    |
| 42  | RW    | 0.30         | 0/911           | 0.51        | 0/1220           |
| 42  | YW    | 0.31         | 0/911           | 0.52        | 0/1220           |
| 43  | RX    | 0.32         | 0/739           | 0.51        | 0/993            |
| 43  | YX    | 0.35         | 0/739           | 0.52        | 0/993            |
| 44  | RY    | 0.33         | 0/798           | 0.61        | 0/1064           |
| 44  | YY    | 0.31         | 0/798           | 0.59        | 0/1064           |
| 45  | RZ    | 0.33         | 0/1435          | 0.58        | 1/1947 (0.1%)    |
| 45  | YZ    | 0.30         | 0/1493          | 0.60        | 0/2026           |
| 46  | R0    | 0.32         | 0/666           | 0.52        | 0/885            |
| 46  | Y0    | 0.32         | 0/666           | 0.58        | 0/885            |
| 47  | R1    | 0.31         | 0/770           | 0.57        | 0/1022           |
| 47  | Y1    | 0.36         | 0/770           | 0.59        | 0/1022           |
| 48  | R2    | 0.28         | 0/583           | 0.58        | 0/771            |
| 48  | Y2    | 0.33         | 0/583           | 0.59        | 1/771 (0.1%)     |
| 49  | R3    | 0.29         | 0/474           | 0.44        | 0/635            |
| 49  | Y3    | 0.28         | 0/474           | 0.47        | 0/635            |
| 50  | R4    | 0.24         | 0/586           | 0.46        | 0/785            |
| 50  | Y4    | 0.30         | 0/586           | 0.50        | 0/785            |
| 51  | R5    | 0.30         | 0/473           | 0.58        | 1/639 (0.2%)     |
| 51  | Y5    | 0.30         | 0/456           | 0.57        | 0/617            |
| 52  | R6    | 0.29         | 0/424           | 0.67        | 0/565            |
| 52  | Y6    | 0.46         | 0/424           | 0.80        | 0/565            |
| 53  | R7    | 0.33         | 0/438           | 0.49        | 0/575            |
| 53  | Y7    | 0.35         | 0/438           | 0.53        | 0/575            |
| 54  | R8    | 0.42         | 0/525           | 0.75        | 0/691            |
| 54  | Y8    | 0.39         | 0/525           | 0.66        | 0/691            |
| 55  | R9    | 0.26         | 0/310           | 0.43        | 0/407            |
| 55  | Y9    | 0.24         | 0/302           | 0.41        | 0/397            |
| All | All   | 0.34         | 7/321792 (0.0%) | 0.76        | 92/481138 (0.0%) |

All (7) bond length outliers are listed below:

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 25  | RA    | 1035 | U    | O3'-P | -5.77 | 1.54        | 1.61     |
| 25  | RA    | 1034 | G    | O3'-P | -5.46 | 1.54        | 1.61     |
| 25  | YA    | 1545 | A    | O3'-P | 5.37  | 1.67        | 1.61     |
| 25  | RA    | 371  | A    | O3'-P | -5.36 | 1.54        | 1.61     |
| 25  | RA    | 2092 | U    | O3'-P | -5.31 | 1.54        | 1.61     |
| 1   | QA    | 349  | A    | O3'-P | -5.14 | 1.54        | 1.61     |
| 12  | XL    | 25   | PRO  | N-CD  | 5.03  | 1.54        | 1.47     |

All (92) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|--------|-------------|----------|
| 31  | YH    | 9      | ILE  | C-N-CD    | -11.87 | 94.49       | 120.60   |
| 1   | XA    | 315    | A    | P-O3'-C3' | 7.69   | 128.93      | 119.70   |
| 25  | RA    | 614(A) | U    | P-O3'-C3' | 7.53   | 128.74      | 119.70   |
| 1   | QA    | 345    | C    | C2-N1-C1' | 7.50   | 127.05      | 118.80   |
| 1   | QA    | 328    | C    | P-O3'-C3' | 6.46   | 127.45      | 119.70   |
| 12  | XL    | 24     | VAL  | C-N-CD    | 5.98   | 140.97      | 128.40   |
| 1   | XA    | 328    | C    | C2-N1-C1' | 5.89   | 125.28      | 118.80   |
| 25  | RA    | 774    | A    | C2-N3-C4  | -5.86  | 107.67      | 110.60   |
| 25  | YA    | 2306   | C    | N1-C2-O2  | 5.84   | 122.40      | 118.90   |
| 35  | YP    | 138    | LEU  | CA-CB-CG  | 5.84   | 128.73      | 115.30   |
| 25  | YA    | 2306   | C    | C2-N1-C1' | 5.81   | 125.19      | 118.80   |
| 25  | YA    | 2848   | G    | P-O3'-C3' | 5.80   | 126.66      | 119.70   |
| 45  | RZ    | 157    | LEU  | C-N-CD    | 5.78   | 140.53      | 128.40   |
| 20  | QT    | 10     | LEU  | CA-CB-CG  | 5.75   | 128.52      | 115.30   |
| 1   | XA    | 328    | C    | P-O3'-C3' | 5.73   | 126.58      | 119.70   |
| 25  | YA    | 1558   | A    | P-O3'-C3' | 5.71   | 126.56      | 119.70   |
| 1   | QA    | 547    | A    | P-O3'-C3' | 5.68   | 126.52      | 119.70   |
| 25  | RA    | 1544   | C    | C2-N1-C1' | 5.68   | 125.05      | 118.80   |
| 25  | RA    | 2275   | C    | C6-N1-C2  | -5.67  | 118.03      | 120.30   |
| 1   | QA    | 971    | G    | C4-N9-C1' | 5.64   | 133.84      | 126.50   |
| 41  | RV    | 35     | LEU  | CA-CB-CG  | 5.63   | 128.24      | 115.30   |
| 1   | QA    | 345    | C    | C6-N1-C1' | -5.62  | 114.05      | 120.80   |
| 25  | YA    | 2439   | A    | P-O3'-C3' | 5.61   | 126.43      | 119.70   |
| 25  | RA    | 2447   | G    | P-O3'-C3' | 5.59   | 126.41      | 119.70   |
| 25  | YA    | 961    | C    | O5'-P-OP1 | -5.55  | 100.70      | 105.70   |
| 1   | XA    | 5      | U    | P-O3'-C3' | 5.55   | 126.36      | 119.70   |
| 1   | XA    | 203    | U    | C2-N1-C1' | 5.54   | 124.35      | 117.70   |
| 25  | RA    | 2275   | C    | P-O3'-C3' | 5.53   | 126.34      | 119.70   |
| 25  | RA    | 1341   | U    | P-O3'-C3' | 5.52   | 126.32      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 25  | YA    | 528  | A    | P-O3'-C3'  | 5.50  | 126.30      | 119.70   |
| 1   | XA    | 197  | A    | P-O3'-C3'  | 5.48  | 126.28      | 119.70   |
| 25  | YA    | 1313 | U    | C2-N1-C1'  | 5.48  | 124.28      | 117.70   |
| 25  | RA    | 1313 | U    | C2-N1-C1'  | 5.48  | 124.27      | 117.70   |
| 25  | YA    | 2287 | A    | C2-N3-C4   | -5.48 | 107.86      | 110.60   |
| 1   | XA    | 687  | A    | P-O3'-C3'  | 5.46  | 126.25      | 119.70   |
| 25  | RA    | 603  | A    | P-O3'-C3'  | 5.45  | 126.24      | 119.70   |
| 1   | XA    | 115  | G    | P-O3'-C3'  | 5.45  | 126.23      | 119.70   |
| 25  | RA    | 587  | C    | P-O3'-C3'  | 5.43  | 126.21      | 119.70   |
| 25  | YA    | 974  | G    | O5'-P-OP2  | -5.42 | 100.82      | 105.70   |
| 25  | RA    | 1544 | C    | N1-C2-O2   | 5.41  | 122.15      | 118.90   |
| 25  | YA    | 1992 | G    | P-O3'-C3'  | 5.41  | 126.19      | 119.70   |
| 1   | QA    | 1065 | U    | P-O3'-C3'  | 5.39  | 126.17      | 119.70   |
| 25  | YA    | 2346 | A    | O4'-C1'-N9 | 5.38  | 112.51      | 108.20   |
| 25  | RA    | 2688 | U    | N3-C2-O2   | -5.38 | 118.43      | 122.20   |
| 1   | QA    | 197  | A    | P-O3'-C3'  | 5.37  | 126.15      | 119.70   |
| 25  | RA    | 1022 | G    | P-O3'-C3'  | 5.34  | 126.11      | 119.70   |
| 25  | YA    | 1022 | G    | P-O3'-C3'  | 5.32  | 126.08      | 119.70   |
| 25  | RA    | 1314 | C    | C5-C6-N1   | 5.31  | 123.66      | 121.00   |
| 1   | QA    | 812  | C    | P-O3'-C3'  | 5.31  | 126.07      | 119.70   |
| 1   | XA    | 792  | A    | P-O3'-C3'  | 5.30  | 126.06      | 119.70   |
| 41  | YV    | 35   | LEU  | CA-CB-CG   | 5.30  | 127.49      | 115.30   |
| 25  | RA    | 2600 | A    | O5'-P-OP1  | -5.29 | 100.94      | 105.70   |
| 35  | YP    | 85   | LEU  | CA-CB-CG   | 5.28  | 127.45      | 115.30   |
| 25  | RA    | 2439 | A    | P-O3'-C3'  | 5.28  | 126.04      | 119.70   |
| 25  | YA    | 748  | G    | O4'-C1'-N9 | 5.28  | 112.42      | 108.20   |
| 25  | YA    | 1653 | G    | P-O3'-C3'  | 5.28  | 126.03      | 119.70   |
| 13  | QM    | 70   | LEU  | CA-CB-CG   | 5.27  | 127.42      | 115.30   |
| 1   | QA    | 913  | A    | P-O3'-C3'  | 5.26  | 126.01      | 119.70   |
| 25  | RA    | 1694 | C    | P-O3'-C3'  | 5.25  | 126.00      | 119.70   |
| 1   | XA    | 530  | G    | N7-C8-N9   | 5.24  | 115.72      | 113.10   |
| 25  | YA    | 1694 | C    | P-O3'-C3'  | 5.23  | 125.98      | 119.70   |
| 25  | YA    | 2211 | G    | P-O3'-C3'  | 5.23  | 125.97      | 119.70   |
| 1   | QA    | 484  | G    | P-O3'-C3'  | 5.22  | 125.96      | 119.70   |
| 25  | RA    | 119  | A    | P-O3'-C3'  | 5.21  | 125.96      | 119.70   |
| 1   | XA    | 818  | G    | P-O3'-C3'  | 5.21  | 125.95      | 119.70   |
| 1   | XA    | 547  | A    | P-O3'-C3'  | 5.20  | 125.94      | 119.70   |
| 2   | XB    | 154  | LEU  | CA-CB-CG   | 5.20  | 127.25      | 115.30   |
| 1   | QA    | 1346 | A    | P-O3'-C3'  | 5.18  | 125.92      | 119.70   |
| 31  | RH    | 9    | ILE  | C-N-CD     | -5.16 | 109.24      | 120.60   |
| 25  | YA    | 2585 | U    | C2-N1-C1'  | 5.16  | 123.89      | 117.70   |
| 48  | Y2    | 16   | LEU  | CA-CB-CG   | 5.16  | 127.16      | 115.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 1   | XA    | 203  | U    | N1-C2-O2   | 5.15 | 126.40      | 122.80   |
| 25  | YA    | 2447 | G    | P-O3'-C3'  | 5.15 | 125.88      | 119.70   |
| 12  | QL    | 47   | LYS  | C-N-CD     | 5.14 | 139.20      | 128.40   |
| 36  | YQ    | 82   | ARG  | N-CA-C     | 5.14 | 124.88      | 111.00   |
| 25  | RA    | 1992 | G    | P-O3'-C3'  | 5.13 | 125.86      | 119.70   |
| 1   | XA    | 913  | A    | P-O3'-C3'  | 5.13 | 125.86      | 119.70   |
| 1   | XA    | 748  | C    | P-O3'-C3'  | 5.09 | 125.81      | 119.70   |
| 1   | XA    | 243  | A    | P-O3'-C3'  | 5.09 | 125.81      | 119.70   |
| 51  | R5    | 4    | HIS  | C-N-CD     | 5.08 | 139.06      | 128.40   |
| 1   | QA    | 687  | A    | P-O3'-C3'  | 5.07 | 125.79      | 119.70   |
| 1   | XA    | 328  | C    | N1-C2-O2   | 5.06 | 121.94      | 118.90   |
| 25  | RA    | 2610 | C    | P-O3'-C3'  | 5.06 | 125.77      | 119.70   |
| 25  | YA    | 119  | A    | P-O3'-C3'  | 5.05 | 125.76      | 119.70   |
| 1   | XA    | 1067 | A    | P-O3'-C3'  | 5.05 | 125.75      | 119.70   |
| 25  | RA    | 1653 | G    | P-O3'-C3'  | 5.04 | 125.75      | 119.70   |
| 1   | QA    | 243  | A    | P-O3'-C3'  | 5.03 | 125.74      | 119.70   |
| 25  | RA    | 227  | A    | P-O3'-C3'  | 5.01 | 125.72      | 119.70   |
| 1   | XA    | 1094 | G    | P-O3'-C3'  | 5.01 | 125.71      | 119.70   |
| 1   | QA    | 60   | A    | P-O3'-C3'  | 5.01 | 125.71      | 119.70   |
| 1   | QA    | 792  | A    | P-O3'-C3'  | 5.01 | 125.71      | 119.70   |
| 25  | YA    | 2278 | A    | O4'-C1'-N9 | 5.01 | 112.20      | 108.20   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | QA    | 32472 | 0        | 16393    | 490     | 0            |
| 1   | XA    | 32409 | 0        | 16361    | 449     | 0            |
| 2   | QB    | 1915  | 0        | 1969     | 56      | 0            |
| 2   | XB    | 1915  | 0        | 1969     | 60      | 0            |
| 3   | QC    | 1612  | 0        | 1677     | 51      | 0            |
| 3   | XC    | 1612  | 0        | 1677     | 50      | 0            |
| 4   | QD    | 1703  | 0        | 1765     | 47      | 0            |
| 4   | XD    | 1703  | 0        | 1765     | 43      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | QE    | 1178  | 0        | 1234     | 29      | 0            |
| 5   | XE    | 1178  | 0        | 1234     | 22      | 0            |
| 6   | QF    | 843   | 0        | 857      | 18      | 0            |
| 6   | XF    | 843   | 0        | 857      | 22      | 0            |
| 7   | QG    | 1257  | 0        | 1296     | 30      | 0            |
| 7   | XG    | 1257  | 0        | 1296     | 35      | 0            |
| 8   | QH    | 1116  | 0        | 1177     | 30      | 0            |
| 8   | XH    | 1116  | 0        | 1177     | 27      | 0            |
| 9   | QI    | 1018  | 0        | 1049     | 52      | 0            |
| 9   | XI    | 1018  | 0        | 1049     | 45      | 0            |
| 10  | QJ    | 801   | 0        | 849      | 35      | 0            |
| 10  | XJ    | 801   | 0        | 849      | 46      | 0            |
| 11  | QK    | 901   | 0        | 926      | 27      | 0            |
| 11  | XK    | 901   | 0        | 926      | 23      | 0            |
| 12  | QL    | 975   | 0        | 1062     | 27      | 0            |
| 12  | XL    | 975   | 0        | 1062     | 24      | 0            |
| 13  | QM    | 937   | 0        | 995      | 27      | 0            |
| 13  | XM    | 937   | 0        | 995      | 56      | 0            |
| 14  | QN    | 492   | 0        | 528      | 15      | 0            |
| 14  | XN    | 492   | 0        | 528      | 20      | 0            |
| 15  | QO    | 734   | 0        | 771      | 14      | 0            |
| 15  | XO    | 734   | 0        | 771      | 14      | 0            |
| 16  | QP    | 705   | 0        | 725      | 15      | 0            |
| 16  | XP    | 705   | 0        | 725      | 9       | 0            |
| 17  | QQ    | 834   | 0        | 904      | 16      | 0            |
| 17  | XQ    | 834   | 0        | 904      | 19      | 0            |
| 18  | QR    | 585   | 0        | 657      | 11      | 0            |
| 18  | XR    | 585   | 0        | 657      | 19      | 0            |
| 19  | QS    | 656   | 0        | 678      | 47      | 0            |
| 19  | XS    | 656   | 0        | 678      | 42      | 0            |
| 20  | QT    | 763   | 0        | 861      | 23      | 0            |
| 20  | XT    | 763   | 0        | 861      | 28      | 0            |
| 21  | QU    | 217   | 0        | 234      | 12      | 0            |
| 21  | XU    | 217   | 0        | 234      | 16      | 0            |
| 22  | QV    | 1640  | 0        | 837      | 29      | 0            |
| 22  | QW    | 1640  | 0        | 837      | 46      | 0            |
| 22  | XV    | 1640  | 0        | 837      | 18      | 0            |
| 22  | XW    | 1640  | 0        | 837      | 23      | 0            |
| 23  | QX    | 440   | 9        | 224      | 18      | 0            |
| 23  | XX    | 440   | 9        | 224      | 15      | 0            |
| 24  | QY    | 746   | 0        | 742      | 16      | 0            |
| 24  | XY    | 746   | 0        | 742      | 17      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25  | RA    | 62269 | 0        | 31392    | 818     | 0            |
| 25  | YA    | 61924 | 0        | 31213    | 687     | 0            |
| 26  | RB    | 2617  | 0        | 1328     | 29      | 0            |
| 26  | YB    | 2617  | 0        | 1328     | 33      | 0            |
| 27  | RD    | 2115  | 0        | 2195     | 66      | 0            |
| 27  | YD    | 2115  | 0        | 2195     | 83      | 0            |
| 28  | RE    | 1568  | 0        | 1634     | 123     | 0            |
| 28  | YE    | 1568  | 0        | 1634     | 79      | 0            |
| 29  | RF    | 1627  | 0        | 1680     | 50      | 0            |
| 29  | YF    | 1627  | 0        | 1680     | 58      | 0            |
| 30  | RG    | 1474  | 0        | 1535     | 49      | 0            |
| 30  | YG    | 1474  | 0        | 1535     | 51      | 0            |
| 31  | RH    | 1307  | 0        | 1382     | 89      | 0            |
| 31  | YH    | 1307  | 0        | 1382     | 66      | 0            |
| 32  | RI    | 1136  | 0        | 1223     | 32      | 0            |
| 32  | YI    | 1136  | 0        | 1223     | 62      | 0            |
| 33  | RN    | 1104  | 0        | 1180     | 14      | 0            |
| 33  | YN    | 1104  | 0        | 1180     | 24      | 0            |
| 34  | RO    | 933   | 0        | 996      | 32      | 0            |
| 34  | YO    | 933   | 0        | 996      | 26      | 0            |
| 35  | RP    | 1145  | 0        | 1228     | 91      | 0            |
| 35  | YP    | 1145  | 0        | 1228     | 97      | 0            |
| 36  | RQ    | 1112  | 0        | 1170     | 33      | 0            |
| 36  | YQ    | 1107  | 0        | 1166     | 40      | 0            |
| 37  | RR    | 960   | 0        | 1021     | 17      | 0            |
| 37  | YR    | 960   | 0        | 1021     | 23      | 0            |
| 38  | RS    | 882   | 0        | 943      | 30      | 0            |
| 38  | YS    | 882   | 0        | 943      | 35      | 0            |
| 39  | RT    | 1141  | 0        | 1202     | 46      | 0            |
| 39  | YT    | 1141  | 0        | 1202     | 36      | 0            |
| 40  | RU    | 964   | 0        | 1022     | 41      | 0            |
| 40  | YU    | 964   | 0        | 1022     | 30      | 0            |
| 41  | RV    | 779   | 0        | 852      | 63      | 0            |
| 41  | YV    | 779   | 0        | 852      | 54      | 0            |
| 42  | RW    | 900   | 0        | 964      | 24      | 0            |
| 42  | YW    | 900   | 0        | 964      | 21      | 0            |
| 43  | RX    | 725   | 0        | 778      | 14      | 0            |
| 43  | YX    | 725   | 0        | 778      | 16      | 0            |
| 44  | RY    | 785   | 0        | 878      | 54      | 0            |
| 44  | YY    | 785   | 0        | 878      | 54      | 0            |
| 45  | RZ    | 1404  | 0        | 1437     | 80      | 0            |
| 45  | YZ    | 1461  | 0        | 1493     | 47      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 46  | R0    | 657   | 0        | 683      | 17      | 0            |
| 46  | Y0    | 657   | 0        | 683      | 25      | 0            |
| 47  | R1    | 763   | 0        | 848      | 31      | 0            |
| 47  | Y1    | 763   | 0        | 848      | 23      | 0            |
| 48  | R2    | 581   | 0        | 629      | 17      | 0            |
| 48  | Y2    | 581   | 0        | 629      | 14      | 0            |
| 49  | R3    | 469   | 0        | 518      | 10      | 0            |
| 49  | Y3    | 469   | 0        | 518      | 9       | 0            |
| 50  | R4    | 573   | 0        | 565      | 25      | 0            |
| 50  | Y4    | 573   | 0        | 565      | 45      | 0            |
| 51  | R5    | 459   | 0        | 480      | 10      | 0            |
| 51  | Y5    | 442   | 0        | 465      | 24      | 0            |
| 52  | R6    | 417   | 0        | 441      | 27      | 0            |
| 52  | Y6    | 417   | 0        | 441      | 46      | 0            |
| 53  | R7    | 430   | 0        | 480      | 6       | 0            |
| 53  | Y7    | 430   | 0        | 480      | 12      | 0            |
| 54  | R8    | 517   | 0        | 582      | 42      | 0            |
| 54  | Y8    | 517   | 0        | 582      | 37      | 0            |
| 55  | R9    | 307   | 0        | 338      | 11      | 0            |
| 55  | Y9    | 299   | 0        | 326      | 6       | 0            |
| 56  | QA    | 150   | 0        | 0        | 0       | 0            |
| 56  | QD    | 2     | 0        | 0        | 0       | 0            |
| 56  | QL    | 1     | 0        | 0        | 0       | 0            |
| 56  | QV    | 4     | 0        | 0        | 0       | 0            |
| 56  | QX    | 1     | 0        | 0        | 0       | 0            |
| 56  | R0    | 3     | 0        | 0        | 0       | 0            |
| 56  | R1    | 1     | 0        | 0        | 0       | 0            |
| 56  | R2    | 1     | 0        | 0        | 0       | 0            |
| 56  | R5    | 3     | 0        | 0        | 0       | 0            |
| 56  | RA    | 441   | 0        | 0        | 0       | 0            |
| 56  | RB    | 4     | 0        | 0        | 0       | 0            |
| 56  | RD    | 2     | 0        | 0        | 0       | 0            |
| 56  | RE    | 1     | 0        | 0        | 0       | 0            |
| 56  | RF    | 1     | 0        | 0        | 0       | 0            |
| 56  | RP    | 3     | 0        | 0        | 0       | 0            |
| 56  | RQ    | 2     | 0        | 0        | 0       | 0            |
| 56  | RR    | 1     | 0        | 0        | 0       | 0            |
| 56  | RT    | 1     | 0        | 0        | 0       | 0            |
| 56  | RV    | 1     | 0        | 0        | 0       | 0            |
| 56  | RY    | 1     | 0        | 0        | 0       | 0            |
| 56  | XA    | 163   | 0        | 0        | 0       | 0            |
| 56  | XD    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56  | XF    | 1      | 0        | 0        | 0       | 0            |
| 56  | XL    | 1      | 0        | 0        | 0       | 0            |
| 56  | XS    | 1      | 0        | 0        | 0       | 0            |
| 56  | XV    | 3      | 0        | 0        | 0       | 0            |
| 56  | Y0    | 3      | 0        | 0        | 0       | 0            |
| 56  | Y1    | 1      | 0        | 0        | 0       | 0            |
| 56  | Y5    | 3      | 0        | 0        | 0       | 0            |
| 56  | Y7    | 1      | 0        | 0        | 0       | 0            |
| 56  | YA    | 487    | 0        | 0        | 0       | 0            |
| 56  | YB    | 6      | 0        | 0        | 0       | 0            |
| 56  | YD    | 1      | 0        | 0        | 0       | 0            |
| 56  | YE    | 1      | 0        | 0        | 0       | 0            |
| 56  | YF    | 1      | 0        | 0        | 0       | 0            |
| 56  | YG    | 1      | 0        | 0        | 0       | 0            |
| 56  | YH    | 1      | 0        | 0        | 0       | 0            |
| 56  | YN    | 1      | 0        | 0        | 0       | 0            |
| 56  | YO    | 1      | 0        | 0        | 0       | 0            |
| 56  | YP    | 1      | 0        | 0        | 0       | 0            |
| 56  | YQ    | 2      | 0        | 0        | 0       | 0            |
| 56  | YV    | 1      | 0        | 0        | 0       | 0            |
| 56  | YW    | 1      | 0        | 0        | 0       | 0            |
| 56  | YY    | 1      | 0        | 0        | 0       | 0            |
| 57  | QD    | 1      | 0        | 0        | 0       | 0            |
| 57  | QN    | 1      | 0        | 0        | 0       | 0            |
| 57  | XD    | 1      | 0        | 0        | 0       | 0            |
| 57  | XN    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 297531 | 18       | 201516   | 5344    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (5344) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 41:YV:49:THR:CG2 | 41:YV:50:PRO:HD3  | 1.35                     | 1.56              |
| 44:RY:76:CYS:SG  | 44:RY:77:PRO:HD2  | 1.44                     | 1.55              |
| 31:RH:9:ILE:CG2  | 31:RH:10:PRO:HA   | 1.36                     | 1.51              |
| 41:RV:49:THR:CG2 | 41:RV:50:PRO:HD3  | 1.50                     | 1.41              |
| 32:YI:77:LEU:HB2 | 32:YI:142:VAL:CG2 | 1.54                     | 1.37              |
| 32:YI:78:THR:H   | 32:YI:142:VAL:CG2 | 1.39                     | 1.35              |
| 50:Y4:6:HIS:HB2  | 50:Y4:7:PRO:CD    | 1.37                     | 1.34              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:XC:3:ASN:O      | 3:XC:4:LYS:HG3     | 1.26                     | 1.32              |
| 41:YV:49:THR:CB   | 41:YV:50:PRO:HD3   | 1.57                     | 1.32              |
| 28:RE:78:LEU:HD23 | 28:RE:79:ARG:CG    | 1.59                     | 1.31              |
| 31:RH:9:ILE:HB    | 31:RH:10:PRO:CB    | 1.61                     | 1.31              |
| 13:XM:8:GLU:O     | 13:XM:9:ILE:HG22   | 1.09                     | 1.26              |
| 32:YI:78:THR:N    | 32:YI:142:VAL:HG23 | 1.52                     | 1.25              |
| 51:Y5:4:HIS:HB3   | 51:Y5:5:PRO:CD     | 1.61                     | 1.24              |
| 1:XA:1157:A:O2'   | 1:XA:1158:C:H5''   | 1.34                     | 1.24              |
| 28:RE:78:LEU:CD2  | 28:RE:79:ARG:CG    | 2.15                     | 1.24              |
| 35:RP:60:MET:O    | 35:RP:61:ARG:HG2   | 1.37                     | 1.23              |
| 1:XA:1158:C:H3'   | 1:XA:1158:C:O2     | 1.40                     | 1.20              |
| 35:RP:59:LEU:HD22 | 54:R8:59:LYS:NZ    | 1.56                     | 1.20              |
| 35:YP:62:LEU:HD12 | 54:Y8:25:MET:O     | 1.39                     | 1.19              |
| 44:YY:76:CYS:SG   | 44:YY:77:PRO:HD2   | 1.83                     | 1.19              |
| 44:RY:76:CYS:SG   | 44:RY:77:PRO:CD    | 2.30                     | 1.18              |
| 45:YZ:155:LEU:O   | 45:YZ:155:LEU:HD12 | 1.42                     | 1.16              |
| 28:RE:78:LEU:CD2  | 28:RE:79:ARG:HG3   | 1.74                     | 1.15              |
| 32:YI:77:LEU:HD12 | 32:YI:142:VAL:HG21 | 1.22                     | 1.15              |
| 41:YV:49:THR:HG22 | 41:YV:50:PRO:CD    | 1.75                     | 1.15              |
| 41:RV:49:THR:HB   | 41:RV:50:PRO:HD2   | 1.20                     | 1.14              |
| 51:Y5:4:HIS:CB    | 51:Y5:5:PRO:HD3    | 1.78                     | 1.13              |
| 30:YG:67:LYS:H    | 50:Y4:6:HIS:CD2    | 1.65                     | 1.13              |
| 31:RH:9:ILE:HG22  | 31:RH:10:PRO:CA    | 1.78                     | 1.13              |
| 45:RZ:59:LEU:O    | 45:RZ:60:GLU:HG3   | 1.48                     | 1.11              |
| 41:RV:49:THR:HB   | 41:RV:50:PRO:CD    | 1.79                     | 1.10              |
| 50:Y4:6:HIS:CB    | 50:Y4:7:PRO:HD3    | 1.80                     | 1.10              |
| 50:Y4:6:HIS:CB    | 50:Y4:7:PRO:CD     | 2.30                     | 1.10              |
| 41:RV:49:THR:CB   | 41:RV:50:PRO:CD    | 2.30                     | 1.10              |
| 13:XM:9:ILE:HG13  | 13:XM:10:PRO:HD2   | 1.33                     | 1.10              |
| 13:XM:8:GLU:O     | 13:XM:9:ILE:CG2    | 1.97                     | 1.10              |
| 45:RZ:59:LEU:CG   | 45:RZ:60:GLU:H     | 1.65                     | 1.10              |
| 31:RH:9:ILE:HB    | 31:RH:10:PRO:CA    | 1.82                     | 1.10              |
| 41:RV:49:THR:HG22 | 41:RV:50:PRO:CD    | 1.82                     | 1.09              |
| 28:RE:63:LEU:HD12 | 28:RE:64:LYS:H     | 1.16                     | 1.09              |
| 31:RH:9:ILE:CG2   | 31:RH:10:PRO:CA    | 2.30                     | 1.09              |
| 41:RV:49:THR:CG2  | 41:RV:50:PRO:CD    | 2.30                     | 1.09              |
| 25:RA:2446:G:C2'  | 25:RA:2447:G:H5''  | 1.82                     | 1.09              |
| 41:YV:49:THR:CB   | 41:YV:50:PRO:CD    | 2.30                     | 1.09              |
| 31:RH:9:ILE:CB    | 31:RH:10:PRO:HA    | 1.80                     | 1.09              |
| 45:RZ:155:LEU:O   | 45:RZ:156:LYS:HG2  | 1.53                     | 1.08              |
| 1:QA:1490:C:H2'   | 1:QA:1491:G:H5'    | 1.33                     | 1.08              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:RH:9:ILE:CB    | 31:RH:10:PRO:CA    | 2.30                     | 1.07              |
| 28:RE:78:LEU:HD23 | 28:RE:79:ARG:HG3   | 1.08                     | 1.07              |
| 25:RA:2701:C:H3'  | 25:RA:2702:U:H5''  | 1.35                     | 1.07              |
| 45:RZ:59:LEU:HG   | 45:RZ:60:GLU:H     | 1.17                     | 1.07              |
| 45:RZ:157:LEU:O   | 45:RZ:161:VAL:HB   | 1.55                     | 1.06              |
| 41:YV:49:THR:CG2  | 41:YV:50:PRO:CD    | 2.30                     | 1.05              |
| 28:YE:60:ASN:C    | 28:YE:62:PRO:HD2   | 1.76                     | 1.05              |
| 41:YV:49:THR:HB   | 41:YV:50:PRO:CD    | 1.87                     | 1.05              |
| 25:RA:2446:G:H2'  | 25:RA:2447:G:C5'   | 1.86                     | 1.04              |
| 32:RI:125:GLU:HA  | 32:RI:141:LYS:HB3  | 1.36                     | 1.04              |
| 32:YI:77:LEU:CB   | 32:YI:142:VAL:HG22 | 1.86                     | 1.04              |
| 31:RH:9:ILE:HB    | 31:RH:10:PRO:HB3   | 1.08                     | 1.03              |
| 1:QA:1158:C:O2    | 1:QA:1158:C:H2'    | 1.57                     | 1.03              |
| 41:RV:47:VAL:HG22 | 41:RV:47:VAL:O     | 1.56                     | 1.03              |
| 41:YV:49:THR:HG22 | 41:YV:50:PRO:HD3   | 1.06                     | 1.02              |
| 30:RG:60:LEU:HD23 | 30:RG:68:PRO:HB3   | 1.39                     | 1.02              |
| 25:RA:1301:A:O2'  | 25:RA:1302:A:H3'   | 1.56                     | 1.02              |
| 35:YP:61:ARG:O    | 35:YP:62:LEU:HB2   | 1.53                     | 1.02              |
| 3:XC:3:ASN:O      | 3:XC:4:LYS:CG      | 2.08                     | 1.02              |
| 41:RV:49:THR:HG22 | 41:RV:50:PRO:HD3   | 1.02                     | 1.01              |
| 32:YI:141:LYS:HB3 | 32:YI:142:VAL:HG22 | 1.40                     | 1.00              |
| 28:YE:63:LEU:O    | 28:YE:64:LYS:HB2   | 1.57                     | 1.00              |
| 25:RA:2446:G:H2'  | 25:RA:2447:G:H5'   | 1.40                     | 1.00              |
| 32:YI:144:VAL:O   | 32:YI:145:VAL:HG12 | 1.62                     | 0.99              |
| 31:RH:7:LEU:HD11  | 31:RH:66:GLY:HA2   | 1.43                     | 0.99              |
| 45:RZ:59:LEU:HD12 | 45:RZ:60:GLU:N     | 1.77                     | 0.99              |
| 28:RE:78:LEU:CD2  | 28:RE:79:ARG:HG2   | 1.91                     | 0.99              |
| 45:RZ:59:LEU:C    | 45:RZ:60:GLU:HG3   | 1.74                     | 0.99              |
| 25:RA:1224:C:H4'  | 41:RV:85:LYS:HB2   | 1.42                     | 0.99              |
| 7:QG:86:GLN:NE2   | 22:QW:31:G:H21     | 1.61                     | 0.99              |
| 28:RE:47:VAL:HG12 | 28:RE:49:LEU:CD1   | 1.93                     | 0.98              |
| 35:RP:60:MET:C    | 35:RP:61:ARG:HG2   | 1.77                     | 0.98              |
| 35:RP:9:ASN:HB2   | 35:RP:10:PRO:HD2   | 1.46                     | 0.98              |
| 1:QA:1490:C:C2'   | 1:QA:1491:G:H5'    | 1.94                     | 0.98              |
| 10:XJ:49:VAL:HG13 | 14:YN:41:ARG:HD2   | 1.43                     | 0.97              |
| 35:RP:59:LEU:HD13 | 54:R8:56:GLU:HG3   | 1.45                     | 0.97              |
| 25:RA:1548:C:C2   | 25:RA:1549:C:C5    | 2.53                     | 0.97              |
| 45:YZ:121:HIS:H   | 45:YZ:171:ILE:HG13 | 1.28                     | 0.96              |
| 1:XA:1158:C:O2    | 1:XA:1158:C:C3'    | 2.12                     | 0.96              |
| 25:RA:68:G:H3'    | 25:RA:69:C:O2      | 1.65                     | 0.96              |
| 47:Y1:87:PRO:HA   | 47:Y1:90:ILE:HG22  | 1.45                     | 0.95              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:YY:76:CYS:CB   | 44:YY:77:PRO:HD2   | 1.96                     | 0.95              |
| 45:RZ:155:LEU:C   | 45:RZ:156:LYS:HG2  | 1.84                     | 0.95              |
| 51:Y5:4:HIS:CB    | 51:Y5:5:PRO:CD     | 2.40                     | 0.94              |
| 35:RP:9:ASN:CB    | 35:RP:10:PRO:HD2   | 1.95                     | 0.94              |
| 52:Y6:28:ARG:HA   | 52:Y6:29:ASN:HB3   | 1.49                     | 0.94              |
| 19:XS:67:VAL:HG21 | 50:Y4:59:PHE:HB3   | 1.47                     | 0.94              |
| 50:Y4:6:HIS:HB2   | 50:Y4:7:PRO:HD2    | 1.50                     | 0.94              |
| 13:XM:9:ILE:CG1   | 13:XM:10:PRO:HD2   | 1.98                     | 0.94              |
| 25:RA:2446:G:C2'  | 25:RA:2447:G:C5'   | 2.44                     | 0.93              |
| 1:QA:353:A:H5'    | 1:QA:353:A:H8      | 1.33                     | 0.93              |
| 25:RA:1496:A:H8   | 25:RA:1577:C:HO2'  | 1.11                     | 0.93              |
| 32:RI:79:ILE:O    | 32:RI:142:VAL:HG21 | 1.69                     | 0.93              |
| 32:YI:77:LEU:CB   | 32:YI:142:VAL:CG2  | 2.46                     | 0.93              |
| 25:RA:2446:G:O2'  | 25:RA:2447:G:H5''  | 1.69                     | 0.93              |
| 1:QA:1302:U:C5    | 13:QM:17:VAL:HG21  | 2.05                     | 0.92              |
| 1:QA:1490:C:H2'   | 1:QA:1491:G:C5'    | 1.99                     | 0.92              |
| 31:RH:8:PRO:C     | 31:RH:9:ILE:HG12   | 1.90                     | 0.92              |
| 23:QX:12:A:H3'    | 23:QX:13:A:H5''    | 1.50                     | 0.91              |
| 32:RI:79:ILE:C    | 32:RI:142:VAL:HG21 | 1.91                     | 0.91              |
| 52:Y6:28:ARG:HD2  | 52:Y6:29:ASN:HB3   | 1.51                     | 0.90              |
| 44:RY:76:CYS:CB   | 44:RY:77:PRO:HD2   | 1.96                     | 0.90              |
| 45:RZ:59:LEU:CD1  | 45:RZ:60:GLU:H     | 1.84                     | 0.90              |
| 32:YI:77:LEU:HB2  | 32:YI:142:VAL:HG22 | 0.92                     | 0.90              |
| 50:Y4:6:HIS:HB2   | 50:Y4:7:PRO:HD3    | 0.91                     | 0.90              |
| 1:QA:1491:G:O2'   | 1:QA:1492:A:H5'    | 1.71                     | 0.90              |
| 30:YG:67:LYS:N    | 50:Y4:6:HIS:HD2    | 1.68                     | 0.90              |
| 41:YV:49:THR:HB   | 41:YV:50:PRO:HD3   | 1.44                     | 0.89              |
| 32:YI:78:THR:H    | 32:YI:142:VAL:HG23 | 0.72                     | 0.89              |
| 44:YY:76:CYS:SG   | 44:YY:77:PRO:CD    | 2.60                     | 0.89              |
| 35:RP:59:LEU:HD22 | 54:R8:59:LYS:HZ1   | 1.33                     | 0.88              |
| 5:QE:50:GLU:HG3   | 5:QE:52:PRO:HD2    | 1.55                     | 0.88              |
| 32:YI:77:LEU:CD1  | 32:YI:142:VAL:HG21 | 2.03                     | 0.88              |
| 9:QI:11:LYS:HD2   | 9:QI:107:ARG:O     | 1.73                     | 0.88              |
| 45:RZ:58:VAL:O    | 45:RZ:59:LEU:HG    | 1.73                     | 0.88              |
| 32:YI:141:LYS:HB3 | 32:YI:142:VAL:CG2  | 2.04                     | 0.88              |
| 45:YZ:148:ASP:HB3 | 45:YZ:149:SER:HA   | 1.56                     | 0.88              |
| 25:YA:987:G:H2'   | 25:YA:988:A:H5'    | 1.54                     | 0.88              |
| 45:RZ:59:LEU:CG   | 45:RZ:60:GLU:N     | 2.36                     | 0.88              |
| 45:RZ:59:LEU:CD1  | 45:RZ:60:GLU:N     | 2.35                     | 0.87              |
| 44:RY:17:SER:HB2  | 44:RY:71:LYS:HE2   | 1.56                     | 0.87              |
| 35:RP:63:PRO:HB3  | 54:R8:13:ARG:HG2   | 1.55                     | 0.87              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:857:C:H4'   | 46:R0:23:VAL:HG21  | 1.57                     | 0.87              |
| 25:YA:2777:G:H5'' | 25:YA:2778:A:H5'   | 1.54                     | 0.87              |
| 31:RH:9:ILE:CB    | 31:RH:10:PRO:HB3   | 2.01                     | 0.86              |
| 7:QG:77:SER:OG    | 22:QW:32:C:H4'     | 1.75                     | 0.86              |
| 1:QA:1490:C:C2'   | 1:QA:1491:G:C5'    | 2.52                     | 0.86              |
| 25:YA:1496:A:H8   | 25:YA:1577:C:HO2'  | 1.18                     | 0.86              |
| 32:YI:77:LEU:HD12 | 32:YI:142:VAL:CG2  | 2.05                     | 0.86              |
| 45:YZ:155:LEU:O   | 45:YZ:155:LEU:CD1  | 2.22                     | 0.86              |
| 28:RE:48:GLN:O    | 28:RE:49:LEU:HD12  | 1.76                     | 0.86              |
| 32:YI:141:LYS:CB  | 32:YI:142:VAL:HG22 | 2.04                     | 0.86              |
| 11:QK:124:LYS:HD2 | 11:QK:125:PHE:CE1  | 2.10                     | 0.85              |
| 45:RZ:157:LEU:HB3 | 45:RZ:161:VAL:HG11 | 1.56                     | 0.85              |
| 9:QI:10:ARG:HH21  | 9:QI:11:LYS:HD3    | 1.41                     | 0.85              |
| 25:RA:2420:C:H41  | 54:R8:31:HIS:HB3   | 1.38                     | 0.85              |
| 1:XA:1380:U:C5    | 7:XG:2:ALA:O       | 2.29                     | 0.85              |
| 35:RP:57:THR:CG2  | 35:RP:60:MET:HB2   | 2.06                     | 0.85              |
| 28:RE:78:LEU:CG   | 28:RE:79:ARG:HG3   | 2.07                     | 0.85              |
| 39:YT:54:ARG:HA   | 39:YT:59:THR:HB    | 1.57                     | 0.85              |
| 1:QA:664:G:H22    | 1:QA:741:G:H1      | 1.22                     | 0.85              |
| 51:Y5:4:HIS:HB3   | 51:Y5:5:PRO:HD3    | 0.86                     | 0.85              |
| 35:RP:57:THR:HG21 | 35:RP:60:MET:CG    | 2.06                     | 0.85              |
| 19:QS:36:ARG:HD2  | 19:QS:71:LEU:H     | 1.42                     | 0.85              |
| 31:YH:9:ILE:HG22  | 31:YH:10:PRO:HA    | 1.58                     | 0.85              |
| 28:YE:60:ASN:C    | 28:YE:62:PRO:CD    | 2.45                     | 0.84              |
| 52:Y6:28:ARG:HA   | 52:Y6:29:ASN:CB    | 2.07                     | 0.84              |
| 1:XA:353:A:H8     | 1:XA:353:A:H5'     | 1.40                     | 0.84              |
| 1:XA:1191:A:H5'   | 3:XC:4:LYS:CE      | 2.07                     | 0.84              |
| 2:XB:185:ILE:HG22 | 2:XB:199:TYR:HB2   | 1.58                     | 0.84              |
| 22:XV:53:G:O2'    | 22:XV:54:U:H5'     | 1.77                     | 0.84              |
| 1:XA:1502:A:H2    | 1:XA:1505:G:H1     | 1.24                     | 0.84              |
| 31:RH:9:ILE:HG22  | 31:RH:10:PRO:HA    | 0.86                     | 0.84              |
| 35:RP:59:LEU:HD22 | 54:R8:59:LYS:HZ2   | 1.43                     | 0.84              |
| 28:RE:63:LEU:HD12 | 28:RE:64:LYS:N     | 1.92                     | 0.84              |
| 25:RA:2712:U:O2'  | 25:RA:2712(A):A:C8 | 2.30                     | 0.84              |
| 25:RA:2393:A:H5'  | 35:RP:62:LEU:HD23  | 1.60                     | 0.84              |
| 25:RA:1913:A:OP1  | 25:RA:1913:A:H4'   | 1.78                     | 0.83              |
| 1:XA:1493:A:C6    | 25:YA:1913:A:H1'   | 2.12                     | 0.83              |
| 28:YE:63:LEU:O    | 28:YE:64:LYS:CB    | 2.24                     | 0.83              |
| 1:XA:1497:G:H2'   | 1:XA:1498:U:H5'    | 1.60                     | 0.83              |
| 25:YA:273(E):U:H3 | 25:YA:363(A):A:H61 | 1.24                     | 0.83              |
| 25:RA:1300:U:H4'  | 25:RA:1301:A:O5'   | 1.78                     | 0.83              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:YP:52:GLU:HG2  | 35:YP:55:ARG:HE    | 1.42                     | 0.83              |
| 35:YP:62:LEU:HD12 | 54:Y8:25:MET:C     | 1.99                     | 0.83              |
| 25:YA:6:A:C2      | 25:YA:7:G:C4       | 2.67                     | 0.83              |
| 25:YA:2712:U:O2'  | 25:YA:2712(A):A:C8 | 2.30                     | 0.83              |
| 54:R8:40:GLU:H    | 54:R8:43:GLN:HG3   | 1.44                     | 0.83              |
| 28:RE:78:LEU:CG   | 28:RE:79:ARG:CG    | 2.57                     | 0.83              |
| 28:RE:78:LEU:HD23 | 28:RE:79:ARG:NE    | 1.94                     | 0.83              |
| 13:XM:10:PRO:CG   | 13:XM:18:ALA:HA    | 2.08                     | 0.83              |
| 25:RA:58:G:H22    | 25:RA:69:C:H5      | 1.25                     | 0.83              |
| 51:R5:4:HIS:HB3   | 51:R5:5:PRO:HD3    | 1.58                     | 0.83              |
| 1:QA:1502:A:H2    | 1:QA:1505:G:H1     | 1.23                     | 0.82              |
| 25:RA:1342:A:H2   | 25:RA:1602:U:H3    | 1.27                     | 0.82              |
| 25:YA:2287:A:H62  | 25:YA:2344:U:H3    | 1.26                     | 0.82              |
| 32:YI:144:VAL:O   | 32:YI:145:VAL:CG1  | 2.26                     | 0.82              |
| 25:YA:242:G:H5''  | 54:Y8:62:LEU:HD13  | 1.61                     | 0.82              |
| 31:YH:7:LEU:HD11  | 31:YH:66:GLY:HA2   | 1.62                     | 0.82              |
| 45:RZ:59:LEU:HG   | 45:RZ:60:GLU:N     | 1.95                     | 0.82              |
| 25:RA:2712:U:O2'  | 25:RA:2712(A):A:H8 | 1.63                     | 0.82              |
| 41:YV:85:LYS:HG3  | 41:YV:87:HIS:H     | 1.44                     | 0.82              |
| 35:RP:57:THR:HG23 | 35:RP:60:MET:HB2   | 1.62                     | 0.82              |
| 4:XD:31:CYS:SG    | 4:XD:32:ALA:N      | 2.52                     | 0.82              |
| 35:RP:60:MET:O    | 35:RP:61:ARG:CG    | 2.26                     | 0.81              |
| 52:Y6:30:THR:HA   | 52:Y6:31:PRO:C     | 2.01                     | 0.81              |
| 44:YY:17:SER:HB2  | 44:YY:71:LYS:HE2   | 1.60                     | 0.81              |
| 28:RE:78:LEU:HD23 | 28:RE:79:ARG:CD    | 2.10                     | 0.81              |
| 45:RZ:58:VAL:HG12 | 45:RZ:60:GLU:HG2   | 1.59                     | 0.81              |
| 25:YA:1204:A:H62  | 25:YA:1241:A:H2    | 1.25                     | 0.81              |
| 32:YI:78:THR:N    | 32:YI:142:VAL:CG2  | 2.25                     | 0.81              |
| 22:QV:2:G:H2'     | 22:QV:3:C:H6       | 1.43                     | 0.81              |
| 35:RP:19:VAL:HG13 | 35:RP:21:ARG:H     | 1.44                     | 0.81              |
| 25:RA:1548:C:H2'  | 25:RA:1549:C:H6    | 1.44                     | 0.81              |
| 25:YA:986:C:H2'   | 25:YA:987:G:H5''   | 1.62                     | 0.81              |
| 25:RA:2701:C:H3'  | 25:RA:2702:U:C5'   | 2.11                     | 0.81              |
| 23:XX:12:A:H3'    | 23:XX:13:A:H5''    | 1.61                     | 0.81              |
| 25:RA:272(I):U:H3 | 25:RA:363(A):A:H61 | 1.29                     | 0.81              |
| 41:YV:5:VAL:HG23  | 41:YV:37:VAL:HG11  | 1.63                     | 0.81              |
| 19:XS:36:ARG:HD2  | 19:XS:71:LEU:H     | 1.44                     | 0.81              |
| 35:RP:59:LEU:HD13 | 54:R8:56:GLU:CG    | 2.11                     | 0.80              |
| 25:YA:2712:U:O2'  | 25:YA:2712(A):A:H8 | 1.64                     | 0.80              |
| 35:YP:62:LEU:CD1  | 54:Y8:25:MET:O     | 2.28                     | 0.80              |
| 25:YA:2343:C:H6   | 25:YA:2343:C:C5'   | 1.95                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:RE:78:LEU:HD23 | 28:RE:79:ARG:HE   | 1.45                     | 0.80              |
| 1:QA:353:A:H5'    | 1:QA:353:A:C8     | 2.17                     | 0.80              |
| 25:YA:986:C:C2'   | 25:YA:987:G:H5''  | 2.11                     | 0.80              |
| 28:RE:50:GLY:HA2  | 28:RE:77:ILE:HA   | 1.64                     | 0.80              |
| 25:RA:1598:C:H5'  | 43:RX:36:LYS:HB3  | 1.64                     | 0.80              |
| 44:RY:97:ARG:HH21 | 44:RY:98:VAL:HB   | 1.45                     | 0.79              |
| 1:QA:1493:A:H2'   | 1:QA:1494:G:H5'   | 1.64                     | 0.79              |
| 25:YA:141:A:H8    | 25:YA:1595:G:H21  | 1.29                     | 0.79              |
| 25:RA:2580:U:H4'  | 28:RE:130:GLY:HA3 | 1.62                     | 0.79              |
| 25:RA:748:G:H2'   | 25:RA:750:A:OP2   | 1.81                     | 0.79              |
| 4:QD:26:CYS:O     | 4:QD:26:CYS:SG    | 2.39                     | 0.79              |
| 50:Y4:6:HIS:ND1   | 50:Y4:6:HIS:N     | 2.30                     | 0.79              |
| 1:QA:1491:G:H2'   | 1:QA:1492:A:C8    | 2.16                     | 0.79              |
| 1:QA:1491:G:O2'   | 1:QA:1492:A:C5'   | 2.30                     | 0.79              |
| 31:YH:8:PRO:O     | 31:YH:10:PRO:HD3  | 1.82                     | 0.79              |
| 25:RA:1695:G:O2'  | 25:RA:1696:G:H5'  | 1.82                     | 0.79              |
| 1:QA:1223:C:H5''  | 1:QA:1224:G:H5''  | 1.65                     | 0.79              |
| 29:RF:3:GLU:HA    | 29:RF:24:LEU:HG   | 1.65                     | 0.79              |
| 25:YA:2103:C:H42  | 25:YA:2186:G:H1   | 1.28                     | 0.79              |
| 4:QD:31:CYS:SG    | 4:QD:32:ALA:N     | 2.56                     | 0.79              |
| 1:QA:960:U:O2     | 1:QA:960:U:H2'    | 1.79                     | 0.79              |
| 30:RG:60:LEU:HD23 | 30:RG:68:PRO:CB   | 2.13                     | 0.79              |
| 10:QJ:79:ARG:HA   | 10:QJ:82:ILE:HB   | 1.64                     | 0.78              |
| 9:XI:10:ARG:HD3   | 9:XI:75:ASP:HB3   | 1.65                     | 0.78              |
| 25:YA:987:G:H2'   | 25:YA:988:A:C5'   | 2.13                     | 0.78              |
| 25:YA:1225:C:H4'  | 41:YV:85:LYS:HB2  | 1.64                     | 0.78              |
| 28:RE:47:VAL:HG12 | 28:RE:48:GLN:O    | 1.82                     | 0.78              |
| 25:RA:1138:G:H21  | 33:RN:106:MET:HE3 | 1.47                     | 0.78              |
| 25:RA:883:G:H1    | 25:RA:893:C:H42   | 1.30                     | 0.78              |
| 32:YI:141:LYS:HB3 | 32:YI:142:VAL:CA  | 2.13                     | 0.78              |
| 1:XA:953:G:H5'    | 1:XA:965:A:H61    | 1.48                     | 0.78              |
| 44:RY:17:SER:OG   | 44:RY:18:GLY:N    | 2.14                     | 0.78              |
| 25:RA:660:G:H21   | 35:RP:12:ALA:HB2  | 1.47                     | 0.78              |
| 1:XA:960:U:O2     | 1:XA:960:U:H2'    | 1.84                     | 0.77              |
| 1:XA:1178:G:H5'   | 9:XI:93:ARG:HH21  | 1.49                     | 0.77              |
| 45:RZ:59:LEU:O    | 45:RZ:60:GLU:CG   | 2.30                     | 0.77              |
| 44:YY:97:ARG:HH21 | 44:YY:98:VAL:HB   | 1.48                     | 0.77              |
| 52:Y6:28:ARG:HB3  | 52:Y6:31:PRO:O    | 1.85                     | 0.77              |
| 35:YP:9:ASN:CB    | 35:YP:10:PRO:HD2  | 2.14                     | 0.77              |
| 1:QA:1491:G:H21   | 25:RA:1913:A:H61  | 1.30                     | 0.77              |
| 44:YY:19:LYS:HE3  | 44:YY:71:LYS:HZ1  | 1.49                     | 0.77              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:RZ:58:VAL:O     | 45:RZ:59:LEU:CG   | 2.32                     | 0.77              |
| 22:XV:54:U:C2'     | 22:XV:55:U:H5'    | 2.13                     | 0.77              |
| 15:QO:39:LEU:HD12  | 15:QO:56:LEU:HB2  | 1.67                     | 0.77              |
| 25:YA:987:G:C2'    | 25:YA:988:A:H5'   | 2.15                     | 0.77              |
| 12:XL:53:ARG:HG3   | 12:XL:93:LEU:HD21 | 1.67                     | 0.76              |
| 40:RU:92:ARG:HD2   | 40:RU:94:ASN:HB3  | 1.67                     | 0.76              |
| 25:YA:2580:U:H4'   | 28:YE:130:GLY:HA3 | 1.66                     | 0.76              |
| 1:QA:1346:A:H4'    | 1:QA:1347:G:O5'   | 1.85                     | 0.76              |
| 1:QA:1346:A:H4'    | 1:QA:1347:G:C5'   | 2.14                     | 0.76              |
| 25:RA:593:G:H4'    | 54:R8:61:LEU:HD22 | 1.67                     | 0.76              |
| 28:RE:48:GLN:O     | 28:RE:49:LEU:CD1  | 2.33                     | 0.76              |
| 29:RF:4:VAL:HA     | 29:RF:19:GLU:HB3  | 1.67                     | 0.76              |
| 36:RQ:75:THR:HA    | 36:RQ:89:ASN:H    | 1.49                     | 0.76              |
| 54:R8:56:GLU:HA    | 54:R8:59:LYS:HE2  | 1.67                     | 0.76              |
| 22:XV:54:U:O2'     | 22:XV:55:U:H5'    | 1.86                     | 0.76              |
| 45:RZ:156:LYS:C    | 45:RZ:158:PRO:HD3 | 2.06                     | 0.76              |
| 2:QB:77:ALA:HB2    | 2:QB:211:ILE:HD13 | 1.67                     | 0.76              |
| 44:YY:102:CYS:SG   | 44:YY:103:GLY:N   | 2.59                     | 0.76              |
| 13:QM:87:TYR:HB3   | 19:QS:73:GLU:HG2  | 1.67                     | 0.76              |
| 5:XE:50:GLU:HG3    | 5:XE:52:PRO:HD2   | 1.66                     | 0.76              |
| 25:RA:242:G:H5''   | 54:R8:62:LEU:HD13 | 1.68                     | 0.76              |
| 1:QA:1492:A:N3     | 25:RA:1913:A:C2   | 2.54                     | 0.76              |
| 27:YD:206:LEU:HD22 | 27:YD:211:ARG:HG2 | 1.66                     | 0.76              |
| 29:YF:4:VAL:HA     | 29:YF:19:GLU:HB3  | 1.66                     | 0.76              |
| 25:RA:143:G:H4'    | 43:RX:35:THR:HG21 | 1.68                     | 0.75              |
| 35:RP:57:THR:HG21  | 35:RP:60:MET:HG3  | 1.69                     | 0.75              |
| 54:R8:30:ARG:O     | 54:R8:31:HIS:ND1  | 2.20                     | 0.75              |
| 35:RP:125:VAL:HG13 | 35:RP:144:GLU:HB3 | 1.68                     | 0.75              |
| 31:YH:11:VAL:HG23  | 31:YH:13:LYS:HG2  | 1.66                     | 0.75              |
| 28:RE:78:LEU:HG    | 28:RE:79:ARG:CG   | 2.16                     | 0.75              |
| 25:YA:2306:C:H5'   | 25:YA:2307:G:H2'  | 1.67                     | 0.75              |
| 28:RE:78:LEU:CD2   | 28:RE:79:ARG:HE   | 1.99                     | 0.75              |
| 30:RG:60:LEU:HD21  | 30:RG:92:VAL:HG12 | 1.66                     | 0.75              |
| 1:QA:328:C:H4'     | 1:QA:329:A:O5'    | 1.86                     | 0.75              |
| 45:RZ:118:GLN:HG3  | 45:RZ:173:ALA:H   | 1.49                     | 0.75              |
| 1:XA:1493:A:C2'    | 1:XA:1494:G:H5'   | 2.16                     | 0.75              |
| 40:YU:95:LEU:HD13  | 41:YV:4:ILE:HG13  | 1.69                     | 0.75              |
| 25:YA:818:G:HO2'   | 25:YA:838:C:HO2'  | 1.32                     | 0.75              |
| 44:RY:95:LYS:NZ    | 44:RY:96:ILE:O    | 2.20                     | 0.75              |
| 25:RA:1548:C:H2'   | 25:RA:1549:C:C6   | 2.22                     | 0.75              |
| 32:YI:141:LYS:HB3  | 32:YI:142:VAL:CB  | 2.17                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:RE:38:THR:HG22 | 28:RE:40:GLU:H    | 1.51                     | 0.74              |
| 5:XE:71:LEU:HD11  | 5:XE:114:GLY:HA3  | 1.69                     | 0.74              |
| 43:RX:35:THR:HG22 | 43:RX:37:THR:H    | 1.52                     | 0.74              |
| 40:YU:90:VAL:HG22 | 41:YV:39:LEU:HB3  | 1.69                     | 0.74              |
| 25:RA:910:A:H62   | 36:RQ:12:GLN:HA   | 1.49                     | 0.74              |
| 1:QA:1086:U:H3    | 1:QA:1099:G:H22   | 1.35                     | 0.74              |
| 19:QS:67:VAL:HG21 | 50:R4:59:PHE:HB3  | 1.69                     | 0.74              |
| 2:QB:8:LYS:HB3    | 2:QB:217:ARG:HD3  | 1.69                     | 0.74              |
| 37:RR:33:ARG:HG2  | 37:RR:115:GLU:HG2 | 1.69                     | 0.74              |
| 25:RA:1981:A:H5'' | 25:RA:1982:C:OP2  | 1.88                     | 0.74              |
| 31:RH:7:LEU:HD22  | 31:RH:69:ARG:HG2  | 1.69                     | 0.74              |
| 44:YY:95:LYS:NZ   | 44:YY:99:CYS:O    | 2.21                     | 0.74              |
| 10:QJ:79:ARG:NE   | 9:XI:94:ALA:O     | 2.21                     | 0.74              |
| 25:RA:833:U:O2    | 35:RP:55:ARG:NH1  | 2.21                     | 0.74              |
| 25:YA:857:C:OP2   | 46:Y0:77:ARG:NH2  | 2.21                     | 0.74              |
| 22:QW:54:U:H3     | 22:QW:58:A:H62    | 1.34                     | 0.74              |
| 2:QB:54:THR:HG21  | 2:QB:201:ILE:HD11 | 1.70                     | 0.74              |
| 12:XL:25:PRO:HD2  | 12:XL:98:TYR:OH   | 1.87                     | 0.74              |
| 40:YU:92:ARG:HD2  | 40:YU:94:ASN:HB3  | 1.70                     | 0.73              |
| 38:YS:106:ARG:NH1 | 38:YS:106:ARG:O   | 2.21                     | 0.73              |
| 35:RP:14:LYS:O    | 35:RP:16:ARG:N    | 2.21                     | 0.73              |
| 22:QV:54:U:C2'    | 22:QV:55:U:H5'    | 2.18                     | 0.73              |
| 27:YD:44:ASN:HB3  | 27:YD:49:ILE:HA   | 1.68                     | 0.73              |
| 38:RS:62:LYS:HB3  | 38:RS:97:ARG:HD3  | 1.71                     | 0.73              |
| 39:RT:55:ASN:H    | 39:RT:59:THR:HB   | 1.52                     | 0.73              |
| 27:YD:85:ASP:HB2  | 27:YD:92:ILE:HD13 | 1.71                     | 0.73              |
| 52:Y6:28:ARG:CD   | 52:Y6:29:ASN:HB3  | 2.18                     | 0.73              |
| 11:QK:124:LYS:HZ2 | 11:QK:125:PHE:HE1 | 1.35                     | 0.73              |
| 1:XA:1305:G:H22   | 1:XA:1331:G:H2'   | 1.52                     | 0.73              |
| 25:RA:1254:A:H5'  | 25:RA:1255:U:H5'  | 1.70                     | 0.73              |
| 35:YP:61:ARG:O    | 35:YP:62:LEU:CB   | 2.35                     | 0.73              |
| 1:QA:350:G:H8     | 1:QA:350:G:C5'    | 2.02                     | 0.73              |
| 52:Y6:6:ARG:HG2   | 52:Y6:8:LYS:H     | 1.52                     | 0.73              |
| 23:QX:14:A:C2'    | 23:QX:15:A:H5'    | 2.19                     | 0.73              |
| 2:QB:48:MET:HA    | 2:QB:51:LEU:HD12  | 1.71                     | 0.73              |
| 1:XA:677:U:H3     | 1:XA:713:G:H22    | 1.35                     | 0.73              |
| 25:YA:1138:G:H21  | 33:YN:106:MET:HE3 | 1.52                     | 0.73              |
| 47:R1:83:GLU:HG2  | 47:R1:85:LEU:H    | 1.52                     | 0.73              |
| 25:RA:1169:G:H1   | 25:RA:1180:C:H42  | 1.37                     | 0.73              |
| 25:YA:1981:A:H5'' | 25:YA:1982:C:OP2  | 1.88                     | 0.73              |
| 28:RE:78:LEU:HD21 | 28:RE:79:ARG:HG2  | 1.70                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:986:C:H2'    | 25:YA:987:G:C5'    | 2.18                     | 0.73              |
| 25:YA:2294:C:OP1   | 38:YS:89:ARG:NH2   | 2.22                     | 0.73              |
| 25:RA:1548:C:O2'   | 25:RA:1549:C:H5'   | 1.88                     | 0.72              |
| 35:YP:14:LYS:O     | 35:YP:16:ARG:N     | 2.22                     | 0.72              |
| 1:XA:530:G:C4      | 23:XX:21:A2M:H2    | 2.24                     | 0.72              |
| 25:RA:655:A:H4'    | 25:RA:656:G:H5'    | 1.71                     | 0.72              |
| 25:YA:259:G:H21    | 25:YA:621:A:H8     | 1.37                     | 0.72              |
| 9:QI:27:THR:OG1    | 9:QI:28:VAL:N      | 2.22                     | 0.72              |
| 28:RE:1:MET:N      | 28:RE:200:GLU:OE2  | 2.23                     | 0.72              |
| 47:Y1:83:GLU:HG2   | 47:Y1:85:LEU:H     | 1.54                     | 0.72              |
| 23:QX:12:A:H3'     | 23:QX:13:A:C5'     | 2.20                     | 0.72              |
| 35:YP:9:ASN:HB2    | 35:YP:10:PRO:HD2   | 1.71                     | 0.72              |
| 24:XY:12:LEU:HB3   | 24:XY:18:VAL:HB    | 1.72                     | 0.72              |
| 2:XB:69:LEU:HB3    | 2:XB:162:ILE:HG22  | 1.70                     | 0.72              |
| 37:RR:100:LEU:HD21 | 37:RR:113:LEU:HD13 | 1.71                     | 0.72              |
| 1:XA:1157:A:O2'    | 1:XA:1158:C:C5'    | 2.28                     | 0.72              |
| 29:RF:153:SER:HB2  | 29:RF:190:GLU:H    | 1.55                     | 0.72              |
| 35:YP:62:LEU:CD1   | 54:Y8:25:MET:HB3   | 2.20                     | 0.72              |
| 25:YA:987:G:H5'    | 25:YA:987:G:H8     | 1.54                     | 0.72              |
| 22:QV:2:G:H2'      | 22:QV:3:C:C6       | 2.24                     | 0.72              |
| 19:XS:65:ASN:OD1   | 50:Y4:55:ARG:NH1   | 2.21                     | 0.72              |
| 19:XS:65:ASN:HA    | 50:Y4:55:ARG:HD2   | 1.71                     | 0.72              |
| 34:RO:92:GLU:OE1   | 34:RO:113:LYS:NZ   | 2.22                     | 0.72              |
| 28:RE:47:VAL:HG12  | 28:RE:49:LEU:HD12  | 1.70                     | 0.72              |
| 2:QB:185:ILE:HG22  | 2:QB:199:TYR:HB2   | 1.70                     | 0.72              |
| 25:RA:2134:A:OP2   | 25:RA:2157:G:N2    | 2.23                     | 0.72              |
| 45:YZ:146:ILE:HA   | 45:YZ:174:VAL:HG23 | 1.72                     | 0.72              |
| 52:Y6:28:ARG:CA    | 52:Y6:29:ASN:HB3   | 2.20                     | 0.72              |
| 39:YT:60:THR:HG22  | 39:YT:77:PRO:HA    | 1.72                     | 0.72              |
| 25:RA:613:G:H2'    | 25:RA:614:U:O2     | 1.90                     | 0.72              |
| 35:RP:59:LEU:HD22  | 54:R8:59:LYS:CE    | 2.20                     | 0.72              |
| 22:QW:50:U:H3      | 22:QW:64:G:H1      | 1.38                     | 0.72              |
| 25:YA:1728:G:H8    | 25:YA:1732:A:H62   | 1.38                     | 0.72              |
| 1:QA:591:U:OP2     | 8:QH:30:ARG:NH1    | 2.22                     | 0.72              |
| 25:YA:2781:A:H5''  | 25:YA:2782:G:H5'   | 1.72                     | 0.71              |
| 29:YF:3:GLU:HA     | 29:YF:24:LEU:HG    | 1.70                     | 0.71              |
| 52:Y6:30:THR:N     | 52:Y6:31:PRO:O     | 2.22                     | 0.71              |
| 41:RV:71:LEU:HD11  | 41:RV:83:ARG:HE    | 1.54                     | 0.71              |
| 32:YI:77:LEU:HB3   | 32:YI:141:LYS:HB2  | 1.72                     | 0.71              |
| 4:XD:3:ARG:NE      | 4:XD:118:ARG:HD3   | 2.04                     | 0.71              |
| 45:YZ:150:LEU:HB2  | 45:YZ:171:ILE:HG22 | 1.72                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:Y6:30:THR:CA   | 52:Y6:31:PRO:O     | 2.38                     | 0.71              |
| 1:XA:353:A:C8     | 1:XA:353:A:H5'     | 2.25                     | 0.71              |
| 1:XA:971:G:N2     | 1:XA:1363(A):A:OP2 | 2.23                     | 0.71              |
| 1:XA:255:G:OP1    | 17:XQ:69:LYS:NZ    | 2.21                     | 0.71              |
| 35:YP:62:LEU:CD1  | 54:Y8:25:MET:C     | 2.59                     | 0.71              |
| 25:RA:252:G:OP2   | 35:RP:50:ARG:NH2   | 2.23                     | 0.71              |
| 22:QW:19:G:N1     | 25:RA:2112:G:N2    | 2.38                     | 0.71              |
| 25:RA:1024:G:H3'  | 25:RA:1025:G:H5''  | 1.71                     | 0.71              |
| 1:QA:1491:G:N2    | 25:RA:1913:A:H61   | 1.89                     | 0.71              |
| 54:Y8:14:VAL:HG13 | 54:Y8:24:ALA:HB2   | 1.72                     | 0.71              |
| 1:QA:1346:A:C4'   | 1:QA:1347:G:O5'    | 2.39                     | 0.71              |
| 31:YH:44:VAL:O    | 31:YH:51:ARG:NH1   | 2.24                     | 0.71              |
| 34:RO:25:LEU:HB2  | 34:RO:38:VAL:HG23  | 1.72                     | 0.71              |
| 13:XM:10:PRO:HG3  | 13:XM:18:ALA:HA    | 1.70                     | 0.71              |
| 41:YV:15:GLU:HG3  | 41:YV:16:PRO:HD2   | 1.72                     | 0.71              |
| 25:RA:2420:C:N4   | 54:R8:31:HIS:HB3   | 2.06                     | 0.70              |
| 36:RQ:89:ASN:O    | 36:RQ:91:GLU:N     | 2.24                     | 0.70              |
| 25:RA:2134:A:N6   | 25:RA:2157:G:O2'   | 2.24                     | 0.70              |
| 25:RA:907:U:OP1   | 36:RQ:24:GLY:N     | 2.22                     | 0.70              |
| 1:QA:673:G:H2'    | 1:QA:674:G:C8      | 2.26                     | 0.70              |
| 31:RH:9:ILE:CB    | 31:RH:10:PRO:CB    | 2.53                     | 0.70              |
| 29:RF:24:LEU:HD13 | 29:RF:25:PRO:HD2   | 1.71                     | 0.70              |
| 25:RA:2119:A:N6   | 25:RA:2170:A:N7    | 2.39                     | 0.70              |
| 32:YI:141:LYS:HB3 | 32:YI:142:VAL:HA   | 1.73                     | 0.70              |
| 41:RV:47:VAL:O    | 41:RV:47:VAL:CG2   | 2.30                     | 0.70              |
| 25:RA:1548:C:C4   | 25:RA:1549:C:N4    | 2.59                     | 0.70              |
| 25:RA:58:G:H1     | 25:RA:69:C:H41     | 1.36                     | 0.70              |
| 1:QA:353:A:H8     | 1:QA:353:A:C5'     | 2.02                     | 0.70              |
| 1:XA:1177:G:OP2   | 9:XI:97:LYS:NZ     | 2.24                     | 0.70              |
| 27:YD:35:LYS:HG2  | 27:YD:64:ILE:N     | 2.05                     | 0.70              |
| 20:XT:67:ALA:HA   | 20:XT:73:HIS:H     | 1.57                     | 0.70              |
| 3:XC:84:ILE:HD12  | 3:XC:88:ARG:HH21   | 1.56                     | 0.70              |
| 1:XA:1380:U:H5    | 7:XG:2:ALA:O       | 1.71                     | 0.70              |
| 25:YA:2343:C:H6   | 25:YA:2343:C:H5''  | 1.57                     | 0.70              |
| 36:RQ:89:ASN:O    | 36:RQ:92:GLY:N     | 2.25                     | 0.70              |
| 52:R6:14:THR:OG1  | 52:R6:15:GLU:N     | 2.25                     | 0.70              |
| 25:RA:1171:G:H1   | 25:RA:1178:C:H42   | 1.39                     | 0.70              |
| 1:QA:974:A:OP2    | 14:QN:29:ARG:NH2   | 2.25                     | 0.70              |
| 19:XS:50:ALA:HB1  | 19:XS:57:HIS:HB3   | 1.71                     | 0.70              |
| 25:YA:571:A:H5'   | 25:YA:2030:A:H62   | 1.57                     | 0.70              |
| 28:YE:60:ASN:O    | 28:YE:61:ARG:HB2   | 1.92                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:YE:61:ARG:N    | 28:YE:62:PRO:HD2  | 2.06                     | 0.70              |
| 30:RG:60:LEU:CD2  | 30:RG:68:PRO:HB3  | 2.18                     | 0.70              |
| 19:QS:36:ARG:NH1  | 19:QS:73:GLU:HB2  | 2.06                     | 0.70              |
| 31:YH:17:VAL:HG21 | 31:YH:49:VAL:HG23 | 1.73                     | 0.70              |
| 29:YF:53:THR:HG23 | 29:YF:55:GLY:H    | 1.56                     | 0.70              |
| 23:QX:10:G:H2'    | 23:QX:11:U:H5''   | 1.74                     | 0.70              |
| 34:YO:98:VAL:HG13 | 34:YO:117:LEU:HB3 | 1.73                     | 0.70              |
| 41:YV:49:THR:HG22 | 41:YV:50:PRO:CG   | 2.22                     | 0.70              |
| 4:QD:20:TYR:HA    | 4:QD:26:CYS:SG    | 2.31                     | 0.70              |
| 48:Y2:42:GLY:O    | 48:Y2:44:LEU:N    | 2.25                     | 0.70              |
| 25:YA:389:G:H22   | 35:YP:72:PRO:HD3  | 1.56                     | 0.70              |
| 9:QI:10:ARG:HD3   | 9:QI:75:ASP:HB3   | 1.73                     | 0.70              |
| 17:XQ:26:GLN:HG2  | 17:XQ:37:LYS:HG2  | 1.74                     | 0.70              |
| 11:QK:10:VAL:HG12 | 11:QK:11:LYS:HG2  | 1.71                     | 0.70              |
| 44:YY:50:ARG:HB3  | 44:YY:53:PRO:HG3  | 1.74                     | 0.70              |
| 25:YA:2011:U:C2'  | 25:YA:2012:G:H5'  | 2.22                     | 0.70              |
| 35:YP:29:LYS:HD2  | 35:YP:30:THR:HG23 | 1.74                     | 0.70              |
| 11:QK:54:ARG:NH2  | 22:QW:39:C:O3'    | 2.23                     | 0.70              |
| 12:QL:60:LEU:HD21 | 12:QL:66:VAL:HG22 | 1.72                     | 0.70              |
| 54:R8:54:GLU:HG3  | 54:R8:57:ARG:HH21 | 1.55                     | 0.70              |
| 25:RA:2635:C:H5'' | 28:RE:78:LEU:HD12 | 1.74                     | 0.69              |
| 52:Y6:6:ARG:CD    | 52:Y6:8:LYS:HB3   | 2.22                     | 0.69              |
| 28:RE:63:LEU:CD1  | 28:RE:65:GLY:H    | 2.05                     | 0.69              |
| 1:XA:542:G:OP1    | 4:XD:10:ARG:NH2   | 2.25                     | 0.69              |
| 35:YP:62:LEU:HG   | 54:Y8:27:THR:HG22 | 1.74                     | 0.69              |
| 3:QC:19:GLU:O     | 3:QC:40:ARG:NH2   | 2.25                     | 0.69              |
| 28:RE:63:LEU:HD13 | 28:RE:65:GLY:H    | 1.57                     | 0.69              |
| 35:YP:94:GLU:HG3  | 35:YP:124:LYS:HB3 | 1.73                     | 0.69              |
| 5:QE:11:ILE:HG22  | 5:QE:12:LEU:HG    | 1.74                     | 0.69              |
| 12:QL:53:ARG:HG3  | 12:QL:93:LEU:HD21 | 1.74                     | 0.69              |
| 27:YD:34:VAL:HG22 | 27:YD:35:LYS:HG3  | 1.73                     | 0.69              |
| 1:XA:1001(A):G:N1 | 1:XA:1039:C:N3    | 2.38                     | 0.69              |
| 19:QS:5:LEU:HD13  | 19:QS:9:VAL:HA    | 1.75                     | 0.69              |
| 25:RA:394:A:H2'   | 25:RA:395:U:H5''  | 1.73                     | 0.69              |
| 28:RE:47:VAL:HG23 | 28:RE:84:PHE:O    | 1.92                     | 0.69              |
| 22:QV:53:G:O2'    | 22:QV:54:U:H5'    | 1.92                     | 0.69              |
| 25:RA:1204:A:H62  | 25:RA:1241:A:H2   | 1.38                     | 0.69              |
| 27:YD:25:THR:O    | 27:YD:27:THR:N    | 2.25                     | 0.69              |
| 29:YF:60:SER:OG   | 29:YF:60:SER:O    | 2.06                     | 0.69              |
| 1:XA:1493:A:H2'   | 1:XA:1494:G:H5'   | 1.75                     | 0.69              |
| 1:XA:960:U:OP1    | 24:XY:8:LYS:HE3   | 1.93                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:Y6:6:ARG:HD3   | 52:Y6:8:LYS:HB3    | 1.73                     | 0.69              |
| 25:YA:1728:G:N1   | 25:YA:1730:U:OP2   | 2.25                     | 0.69              |
| 25:RA:136:G:H1    | 25:RA:143(A):C:H42 | 1.41                     | 0.69              |
| 25:YA:2245:U:H5'  | 25:YA:2246:G:H5'   | 1.72                     | 0.69              |
| 30:YG:83:ARG:H    | 30:YG:86:MET:HG3   | 1.58                     | 0.69              |
| 52:R6:9:LEU:H     | 52:R6:27:LYS:HA    | 1.58                     | 0.69              |
| 1:XA:422:C:O2'    | 1:XA:423:G:N2      | 2.26                     | 0.69              |
| 29:RF:53:THR:HG23 | 29:RF:55:GLY:H     | 1.57                     | 0.69              |
| 31:RH:69:ARG:HG3  | 31:RH:70:THR:N     | 2.08                     | 0.69              |
| 28:YE:60:ASN:CA   | 28:YE:62:PRO:HD2   | 2.23                     | 0.69              |
| 42:RW:18:ARG:HD3  | 42:RW:76:VAL:HG13  | 1.75                     | 0.69              |
| 29:YF:103:LYS:HA  | 29:YF:106:ARG:HG3  | 1.75                     | 0.69              |
| 1:QA:345:C:H1'    | 1:QA:346:G:C2      | 2.28                     | 0.69              |
| 32:YI:80:PRO:CB   | 32:YI:143:SER:O    | 2.41                     | 0.69              |
| 43:YX:43:VAL:HG23 | 43:YX:51:VAL:HG21  | 1.74                     | 0.69              |
| 31:YH:158:HIS:HA  | 31:YH:170:ARG:HG2  | 1.75                     | 0.69              |
| 25:RA:2583:G:C2'  | 25:RA:2584:U:H5'   | 2.23                     | 0.69              |
| 25:YA:2751:G:H1'  | 31:YH:4:ILE:HG13   | 1.74                     | 0.69              |
| 22:XV:53:G:C2'    | 22:XV:54:U:H5'     | 2.22                     | 0.68              |
| 17:QQ:45:HIS:HB2  | 17:QQ:65:ILE:HD13  | 1.75                     | 0.68              |
| 38:YS:106:ARG:NH1 | 38:YS:107:GLU:OE2  | 2.23                     | 0.68              |
| 30:RG:16:ARG:HE   | 30:RG:31:VAL:HG11  | 1.57                     | 0.68              |
| 4:QD:13:ARG:O     | 4:QD:15:GLU:N      | 2.26                     | 0.68              |
| 25:YA:747:U:OP1   | 51:Y5:3:LYS:HG2    | 1.93                     | 0.68              |
| 23:XX:20:A2M:N3   | 23:XX:20:A2M:H5''  | 2.08                     | 0.68              |
| 13:XM:3:ARG:O     | 50:Y4:34:GLU:HG3   | 1.93                     | 0.68              |
| 25:YA:2712:U:OP1  | 25:YA:2714:G:H4'   | 1.92                     | 0.68              |
| 25:RA:2602:A:H4'  | 25:RA:2603:G:O5'   | 1.94                     | 0.68              |
| 1:QA:1491:G:C2'   | 1:QA:1492:A:O5'    | 2.41                     | 0.68              |
| 12:XL:117:ARG:HB3 | 12:XL:122:THR:HB   | 1.73                     | 0.68              |
| 25:YA:651:G:H5''  | 54:Y8:18:ALA:HB3   | 1.75                     | 0.68              |
| 30:RG:66:GLN:NE2  | 30:RG:93:THR:O     | 2.26                     | 0.68              |
| 25:RA:2438:U:O3'  | 25:RA:2439:A:H3'   | 1.93                     | 0.68              |
| 25:YA:1300:U:H4'  | 25:YA:1301:A:H5''  | 1.74                     | 0.68              |
| 25:RA:2343:C:C5'  | 25:RA:2343:C:H6    | 2.07                     | 0.68              |
| 12:QL:47:LYS:HB3  | 12:QL:48:PRO:HD3   | 1.76                     | 0.68              |
| 13:XM:8:GLU:C     | 13:XM:9:ILE:HG22   | 2.10                     | 0.68              |
| 25:YA:2228:G:OP1  | 27:YD:261:LYS:NZ   | 2.26                     | 0.68              |
| 34:RO:68:GLU:OE2  | 34:RO:78:ARG:NH1   | 2.26                     | 0.68              |
| 32:RI:110:ASP:OD1 | 32:RI:110:ASP:N    | 2.26                     | 0.68              |
| 25:RA:1614:A:N1   | 42:RW:93:ALA:HB2   | 2.09                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:61:G:H1      | 25:RA:94:C:H42     | 1.42                     | 0.68              |
| 35:YP:62:LEU:HD13  | 54:Y8:25:MET:HB3   | 1.76                     | 0.68              |
| 23:QX:14:A:O2'     | 23:QX:15:A:H5'     | 1.94                     | 0.68              |
| 25:YA:1728:G:N7    | 25:YA:1731:G:N2    | 2.39                     | 0.68              |
| 52:Y6:40:CYS:HB3   | 52:Y6:46:HIS:CE1   | 2.27                     | 0.68              |
| 31:RH:125:VAL:HG22 | 31:RH:126:PRO:HA   | 1.76                     | 0.68              |
| 10:XJ:51:ARG:HB2   | 10:XJ:60:ARG:HA    | 1.73                     | 0.67              |
| 25:RA:2602:A:H4'   | 25:RA:2603:G:C5'   | 2.22                     | 0.67              |
| 4:QD:191:ARG:NH1   | 4:QD:200:GLU:OE1   | 2.27                     | 0.67              |
| 2:QB:115:LEU:HD13  | 2:QB:145:LEU:HB3   | 1.76                     | 0.67              |
| 23:XX:5:A:H2'      | 23:XX:6:G:H8       | 1.60                     | 0.67              |
| 25:YA:2646:C:O5'   | 25:YA:2646:C:H6    | 1.78                     | 0.67              |
| 1:QA:718:G:C8      | 11:QK:116:HIS:HB3  | 2.29                     | 0.67              |
| 3:QC:164:ARG:NH2   | 3:QC:166:GLU:OE2   | 2.27                     | 0.67              |
| 33:YN:125:GLY:HA3  | 33:YN:126:PRO:O    | 1.93                     | 0.67              |
| 1:QA:1346:A:H4'    | 1:QA:1347:G:H5'    | 1.74                     | 0.67              |
| 49:Y3:8:LEU:HD13   | 49:Y3:31:LEU:HD12  | 1.76                     | 0.67              |
| 2:QB:204:ASN:N     | 2:QB:204:ASN:OD1   | 2.24                     | 0.67              |
| 17:XQ:66:SER:O     | 17:XQ:70:ARG:NH1   | 2.26                     | 0.67              |
| 30:YG:161:THR:HG22 | 30:YG:163:ALA:H    | 1.57                     | 0.67              |
| 25:YA:2438:U:O3'   | 25:YA:2439:A:H3'   | 1.94                     | 0.67              |
| 54:R8:56:GLU:N     | 54:R8:56:GLU:OE1   | 2.24                     | 0.67              |
| 1:QA:1491:G:H2'    | 1:QA:1492:A:H8     | 1.58                     | 0.67              |
| 22:QW:33:U:H6      | 22:QW:33:U:O5'     | 1.78                     | 0.67              |
| 28:YE:37:ARG:HG3   | 28:YE:46:ALA:HB3   | 1.77                     | 0.67              |
| 9:XI:27:THR:OG1    | 9:XI:28:VAL:N      | 2.27                     | 0.67              |
| 13:XM:9:ILE:CG1    | 13:XM:10:PRO:CD    | 2.71                     | 0.67              |
| 28:RE:179:GLU:HB3  | 28:RE:181:LEU:HD22 | 1.77                     | 0.67              |
| 25:YA:1309:G:H4'   | 53:Y7:7:PRO:HB2    | 1.77                     | 0.67              |
| 25:RA:1753:G:OP1   | 39:RT:95:ARG:NE    | 2.25                     | 0.67              |
| 30:YG:67:LYS:N     | 50:Y4:6:HIS:CD2    | 2.51                     | 0.67              |
| 1:QA:1060:C:H2'    | 1:QA:1061:G:H8     | 1.60                     | 0.67              |
| 22:XW:54:U:H3      | 22:XW:58:A:H62     | 1.40                     | 0.67              |
| 1:XA:1179:A:H5'    | 9:XI:102:LEU:HD22  | 1.76                     | 0.67              |
| 31:RH:19:VAL:HG13  | 31:RH:43:VAL:HG22  | 1.77                     | 0.67              |
| 31:YH:9:ILE:CG2    | 31:YH:10:PRO:HA    | 2.24                     | 0.67              |
| 25:YA:857:C:H4'    | 46:Y0:23:VAL:HG21  | 1.76                     | 0.67              |
| 52:Y6:12:GLU:HB2   | 52:Y6:22:ALA:HB3   | 1.77                     | 0.67              |
| 1:XA:531:U:OP2     | 24:XY:69:ARG:NH1   | 2.25                     | 0.67              |
| 28:RE:78:LEU:HG    | 28:RE:79:ARG:HA    | 1.77                     | 0.67              |
| 54:Y8:6:THR:HG21   | 54:Y8:63:PRO:HD3   | 1.77                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:XY:90:ASP:O     | 24:XY:91:TYR:HD2   | 1.78                     | 0.67              |
| 12:XL:27:LEU:HD12  | 12:XL:33:ARG:HB2   | 1.77                     | 0.67              |
| 11:XK:54:ARG:NH2   | 22:XW:39:C:O2'     | 2.28                     | 0.67              |
| 10:XJ:79:ARG:HA    | 10:XJ:82:ILE:HB    | 1.77                     | 0.67              |
| 30:RG:161:THR:HG22 | 30:RG:163:ALA:H    | 1.60                     | 0.67              |
| 41:RV:48:GLY:H     | 41:RV:52:VAL:HG22  | 1.61                     | 0.66              |
| 25:YA:1762:A:H4'   | 25:YA:1763:G:OP2   | 1.92                     | 0.66              |
| 36:YQ:89:ASN:O     | 36:YQ:91:GLU:N     | 2.27                     | 0.66              |
| 20:XT:60:GLU:HG3   | 20:XT:81:LYS:HD2   | 1.76                     | 0.66              |
| 54:R8:8:LYS:HB3    | 54:R8:12:LYS:HE3   | 1.77                     | 0.66              |
| 32:YI:141:LYS:CB   | 32:YI:142:VAL:HA   | 2.25                     | 0.66              |
| 28:RE:47:VAL:CG1   | 28:RE:49:LEU:CD1   | 2.71                     | 0.66              |
| 1:QA:1490:C:O2'    | 1:QA:1491:G:C5'    | 2.43                     | 0.66              |
| 10:QJ:8:LEU:HG     | 10:QJ:96:ILE:HG22  | 1.76                     | 0.66              |
| 29:YF:122:LYS:O    | 29:YF:124:LEU:N    | 2.27                     | 0.66              |
| 32:RI:120:ILE:HG22 | 32:RI:122:GLU:H    | 1.60                     | 0.66              |
| 31:YH:80:SER:OG    | 31:YH:81:GLU:N     | 2.29                     | 0.66              |
| 25:YA:2404:C:H1'   | 35:YP:67:MET:HE1   | 1.76                     | 0.66              |
| 31:RH:7:LEU:HD13   | 31:RH:69:ARG:HB3   | 1.77                     | 0.66              |
| 52:R6:15:GLU:OE1   | 52:R6:44:ARG:NH2   | 2.28                     | 0.66              |
| 25:RA:1019:U:HO2'  | 25:RA:1021:A:H2    | 1.44                     | 0.66              |
| 20:QT:75:ASN:N     | 20:QT:75:ASN:OD1   | 2.29                     | 0.66              |
| 32:YI:144:VAL:C    | 32:YI:145:VAL:HG12 | 2.15                     | 0.66              |
| 45:RZ:10:ARG:NH1   | 45:RZ:26:GLY:O     | 2.28                     | 0.66              |
| 1:QA:1030:C:H3'    | 1:QA:1030(A):G:H4' | 1.77                     | 0.66              |
| 25:YA:1007:C:OP1   | 33:YN:35:ARG:NH1   | 2.29                     | 0.66              |
| 22:QV:53:G:H2'     | 22:QV:54:U:C6      | 2.31                     | 0.66              |
| 31:YH:86:GLU:HG3   | 31:YH:165:ALA:HB2  | 1.78                     | 0.66              |
| 3:XC:71:ALA:HA     | 3:XC:106:VAL:HB    | 1.76                     | 0.66              |
| 35:RP:23:PRO:O     | 35:RP:25:SER:N     | 2.28                     | 0.66              |
| 25:YA:833:U:O2     | 35:YP:55:ARG:NH1   | 2.29                     | 0.66              |
| 31:YH:45:VAL:HG23  | 31:YH:49:VAL:HA    | 1.78                     | 0.66              |
| 35:RP:146:VAL:HG22 | 35:RP:147:LEU:HD13 | 1.78                     | 0.66              |
| 36:YQ:18:LYS:HB2   | 36:YQ:98:LYS:HZ1   | 1.60                     | 0.66              |
| 54:R8:14:VAL:HG13  | 54:R8:24:ALA:HB2   | 1.78                     | 0.66              |
| 2:XB:178:ARG:HH12  | 8:XH:68:ARG:HH22   | 1.41                     | 0.66              |
| 30:RG:96:ARG:O     | 30:RG:98:ARG:N     | 2.28                     | 0.66              |
| 25:YA:2287:A:N6    | 25:YA:2344:U:H3    | 1.93                     | 0.66              |
| 44:RY:50:ARG:HB3   | 44:RY:53:PRO:HG3   | 1.78                     | 0.66              |
| 44:RY:33:LYS:HD3   | 44:RY:33:LYS:H     | 1.61                     | 0.66              |
| 1:QA:1490:C:O2'    | 1:QA:1491:G:H5'    | 1.95                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:XD:13:ARG:O      | 4:XD:15:GLU:N      | 2.29                     | 0.66              |
| 25:YA:2011:U:H2'   | 25:YA:2012:G:H5'   | 1.75                     | 0.66              |
| 46:R0:48:GLY:O     | 46:R0:80:HIS:ND1   | 2.29                     | 0.66              |
| 47:R1:51:VAL:HG11  | 47:R1:74:VAL:HG21  | 1.76                     | 0.66              |
| 36:RQ:64:ILE:HG22  | 36:RQ:106:VAL:HG12 | 1.76                     | 0.66              |
| 23:XX:10:G:N2      | 23:XX:11:U:O3'     | 2.29                     | 0.66              |
| 1:XA:1457:G:OP1    | 20:XT:39:LYS:NZ    | 2.23                     | 0.66              |
| 1:QA:189(F):U:O2   | 17:QQ:63:ARG:NH1   | 2.29                     | 0.66              |
| 1:QA:218:C:H5'     | 1:QA:470:C:H42     | 1.59                     | 0.66              |
| 53:Y7:34:ARG:NH1   | 53:Y7:41:ARG:O     | 2.29                     | 0.66              |
| 25:RA:1917:U:O2'   | 25:RA:1918:A:H5'   | 1.96                     | 0.66              |
| 29:YF:132:VAL:HG22 | 29:YF:133:ASN:H    | 1.61                     | 0.66              |
| 1:XA:664:G:H22     | 1:XA:741:G:H1      | 1.42                     | 0.66              |
| 1:XA:954:G:H21     | 1:XA:1227:A:H62    | 1.45                     | 0.65              |
| 29:YF:66:PRO:O     | 29:YF:68:LYS:N     | 2.29                     | 0.65              |
| 44:RY:89:PHE:HB2   | 44:RY:90:LEU:HD22  | 1.78                     | 0.65              |
| 44:RY:88:LYS:O     | 44:RY:90:LEU:N     | 2.27                     | 0.65              |
| 12:QL:117:ARG:HB3  | 12:QL:122:THR:HB   | 1.78                     | 0.65              |
| 49:Y3:39:ASP:OD2   | 49:Y3:44:ARG:NH2   | 2.29                     | 0.65              |
| 2:QB:194:PRO:O     | 2:QB:196:LEU:N     | 2.29                     | 0.65              |
| 38:RS:26:LEU:HB3   | 38:RS:87:PHE:HA    | 1.79                     | 0.65              |
| 28:RE:47:VAL:C     | 28:RE:48:GLN:O     | 2.33                     | 0.65              |
| 2:XB:195:ASP:O     | 8:XH:68:ARG:NH2    | 2.29                     | 0.65              |
| 25:YA:2105:C:H2'   | 25:YA:2106:G:H8    | 1.61                     | 0.65              |
| 1:XA:1191:A:H5'    | 3:XC:4:LYS:HE2     | 1.76                     | 0.65              |
| 28:YE:61:ARG:N     | 28:YE:62:PRO:CD    | 2.59                     | 0.65              |
| 25:RA:1694:C:H4'   | 25:RA:1695:G:O5'   | 1.95                     | 0.65              |
| 1:XA:960:U:H1'     | 1:XA:961:U:OP2     | 1.95                     | 0.65              |
| 44:RY:61:ILE:HG22  | 44:RY:62:GLU:HG3   | 1.78                     | 0.65              |
| 13:XM:97:PRO:HA    | 13:XM:110:ARG:HD3  | 1.79                     | 0.65              |
| 1:XA:189(F):U:O2   | 17:XQ:63:ARG:NH1   | 2.30                     | 0.65              |
| 35:RP:97:PRO:O     | 35:RP:99:LEU:N     | 2.27                     | 0.65              |
| 28:RE:78:LEU:CD2   | 28:RE:79:ARG:NE    | 2.56                     | 0.65              |
| 40:YU:92:ARG:HH22  | 41:YV:10:LYS:HA    | 1.61                     | 0.65              |
| 32:YI:80:PRO:HB3   | 32:YI:143:SER:O    | 1.96                     | 0.65              |
| 1:XA:1442:G:O6     | 1:XA:1442(B):A:N6  | 2.29                     | 0.65              |
| 1:XA:1289:A:OP1    | 21:XU:9:ARG:NH2    | 2.29                     | 0.65              |
| 44:RY:13:VAL:HG21  | 44:RY:72:VAL:HB    | 1.77                     | 0.65              |
| 19:QS:62:ILE:HA    | 19:QS:66:MET:HE1   | 1.77                     | 0.65              |
| 31:RH:10:PRO:O     | 31:RH:11:VAL:CG1   | 2.44                     | 0.65              |
| 32:YI:120:ILE:HG22 | 32:YI:122:GLU:H    | 1.61                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:1316:G:N1    | 1:XA:1319:A:OP2    | 2.27                     | 0.65              |
| 2:XB:43:ASP:HB3   | 2:XB:46:LYS:HB2    | 1.78                     | 0.65              |
| 25:RA:2128:C:N4   | 25:RA:2159:G:O6    | 2.30                     | 0.65              |
| 20:QT:67:ALA:HA   | 20:QT:73:HIS:H     | 1.62                     | 0.65              |
| 13:XM:10:PRO:HG2  | 13:XM:18:ALA:HA    | 1.79                     | 0.65              |
| 22:XV:54:U:H2'    | 22:XV:55:U:H5'     | 1.78                     | 0.65              |
| 25:RA:1021:A:H3'  | 25:RA:1021:A:H8    | 1.60                     | 0.65              |
| 45:RZ:87:ASP:OD2  | 45:RZ:87:ASP:N     | 2.30                     | 0.65              |
| 7:QG:73:MET:HG2   | 7:QG:90:GLU:HA     | 1.79                     | 0.65              |
| 25:YA:2445:G:OP1  | 29:YF:74:ARG:NH2   | 2.28                     | 0.65              |
| 41:YV:49:THR:HB   | 41:YV:50:PRO:HD2   | 1.74                     | 0.65              |
| 44:RY:76:CYS:O    | 44:RY:78:ALA:N     | 2.30                     | 0.65              |
| 52:Y6:30:THR:HA   | 52:Y6:31:PRO:O     | 1.96                     | 0.65              |
| 29:RF:79:GLY:HA2  | 29:RF:86:GLY:HA2   | 1.78                     | 0.65              |
| 28:RE:8:LYS:HB3   | 28:RE:192:ASN:HA   | 1.77                     | 0.65              |
| 26:YB:80:U:H2'    | 26:YB:81:G:H21     | 1.60                     | 0.65              |
| 25:YA:2016:U:H1'  | 51:Y5:6:VAL:CG1    | 2.27                     | 0.65              |
| 48:R2:17:SER:HB2  | 48:R2:18:PRO:HA    | 1.78                     | 0.65              |
| 3:XC:3:ASN:C      | 3:XC:4:LYS:HG3     | 2.13                     | 0.65              |
| 45:RZ:59:LEU:C    | 45:RZ:60:GLU:CG    | 2.55                     | 0.65              |
| 9:XI:28:VAL:HG21  | 9:XI:63:ILE:N      | 2.09                     | 0.65              |
| 1:XA:455:C:H42    | 1:XA:476:G:H1      | 1.44                     | 0.65              |
| 7:XG:15:ASP:HB3   | 7:XG:24:THR:HG22   | 1.79                     | 0.65              |
| 31:RH:8:PRO:O     | 31:RH:9:ILE:CG1    | 2.45                     | 0.65              |
| 41:RV:49:THR:HG21 | 41:RV:50:PRO:HD3   | 1.71                     | 0.65              |
| 1:QA:1302:U:C5    | 13:QM:17:VAL:CG2   | 2.80                     | 0.65              |
| 25:YA:1403:C:H5'' | 25:YA:1471:A:H1'   | 1.79                     | 0.65              |
| 31:YH:24:VAL:HG22 | 31:YH:35:VAL:HB    | 1.79                     | 0.65              |
| 47:Y1:34:THR:HG22 | 47:Y1:36:GLY:H     | 1.61                     | 0.65              |
| 38:YS:26:LEU:HB3  | 38:YS:87:PHE:HA    | 1.77                     | 0.65              |
| 25:RA:1657:C:H2'  | 25:RA:1658:C:H6    | 1.62                     | 0.65              |
| 36:YQ:64:ILE:HG22 | 36:YQ:106:VAL:HG12 | 1.79                     | 0.65              |
| 44:YY:76:CYS:O    | 44:YY:78:ALA:N     | 2.30                     | 0.64              |
| 11:QK:124:LYS:HD2 | 11:QK:125:PHE:CD1  | 2.31                     | 0.64              |
| 22:QV:54:U:H2'    | 22:QV:55:U:H5'     | 1.79                     | 0.64              |
| 27:YD:35:LYS:HD2  | 27:YD:104:TYR:CE1  | 2.32                     | 0.64              |
| 27:RD:171:ASP:OD2 | 27:RD:171:ASP:N    | 2.29                     | 0.64              |
| 3:XC:11:ARG:HE    | 3:XC:180:ALA:HB3   | 1.62                     | 0.64              |
| 28:RE:78:LEU:CG   | 28:RE:79:ARG:HG2   | 2.24                     | 0.64              |
| 25:RA:68:G:C3'    | 25:RA:69:C:O2      | 2.45                     | 0.64              |
| 25:YA:84:A:N1     | 25:YA:98:G:O2'     | 2.23                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:QG:16:LEU:HD23   | 9:QI:41:VAL:HG12   | 1.80                     | 0.64              |
| 1:XA:350:G:C6      | 1:XA:351:G:O6      | 2.50                     | 0.64              |
| 28:YE:80:GLU:O     | 28:YE:82:ARG:N     | 2.30                     | 0.64              |
| 13:XM:99:ARG:O     | 13:XM:101:GLN:NE2  | 2.30                     | 0.64              |
| 33:YN:49:GLY:O     | 33:YN:119:ARG:NH1  | 2.29                     | 0.64              |
| 44:YY:17:SER:OG    | 44:YY:18:GLY:N     | 2.28                     | 0.64              |
| 27:YD:39:LYS:HB2   | 27:YD:62:TYR:HB2   | 1.78                     | 0.64              |
| 25:RA:271(P):C:H5' | 32:RI:45:LYS:HE3   | 1.79                     | 0.64              |
| 28:RE:63:LEU:CD1   | 28:RE:64:LYS:H     | 2.02                     | 0.64              |
| 1:QA:1491:G:H2'    | 1:QA:1492:A:O5'    | 1.98                     | 0.64              |
| 27:YD:44:ASN:OD1   | 27:YD:44:ASN:N     | 2.29                     | 0.64              |
| 25:YA:1247:A:OP1   | 29:YF:95:ARG:NH2   | 2.30                     | 0.64              |
| 9:QI:34:ASN:O      | 9:QI:36:TYR:N      | 2.30                     | 0.64              |
| 4:XD:148:VAL:HG11  | 4:XD:158:ILE:HG21  | 1.79                     | 0.64              |
| 4:XD:23:GLY:O      | 4:XD:24:GLU:HB2    | 1.97                     | 0.64              |
| 1:XA:673:G:H2'     | 1:XA:674:G:C8      | 2.33                     | 0.64              |
| 1:QA:1318:A:H4'    | 19:QS:10:PHE:CE2   | 2.33                     | 0.64              |
| 7:XG:35:LYS:HB3    | 7:XG:38:LEU:HD13   | 1.79                     | 0.64              |
| 29:YF:135:LYS:HB3  | 29:YF:138:GLU:HG3  | 1.79                     | 0.64              |
| 13:XM:67:GLU:OE2   | 30:YG:115:ARG:NH2  | 2.30                     | 0.64              |
| 45:YZ:121:HIS:N    | 45:YZ:171:ILE:HG13 | 2.08                     | 0.64              |
| 25:RA:2788:C:O2'   | 25:RA:2809:A:N3    | 2.30                     | 0.64              |
| 4:XD:109:GLY:O     | 4:XD:111:ALA:N     | 2.30                     | 0.64              |
| 42:RW:65:LEU:HD13  | 42:RW:68:ARG:HD2   | 1.79                     | 0.64              |
| 25:RA:2091:U:O2'   | 47:R1:47:GLN:HG3   | 1.97                     | 0.64              |
| 2:XB:111:ARG:HA    | 2:XB:111:ARG:HH11  | 1.63                     | 0.64              |
| 25:YA:458:G:C8     | 53:Y7:37:LYS:HG2   | 2.32                     | 0.64              |
| 25:YA:1171:G:H1    | 25:YA:1178:C:H42   | 1.46                     | 0.64              |
| 14:QN:12:ARG:HG2   | 14:QN:14:PRO:HD3   | 1.79                     | 0.64              |
| 28:RE:47:VAL:HG21  | 28:RE:86:PRO:HD2   | 1.78                     | 0.64              |
| 23:XX:13:A:O2'     | 23:XX:14:A:H5''    | 1.98                     | 0.64              |
| 35:RP:52:GLU:OE1   | 35:RP:54:GLY:N     | 2.20                     | 0.64              |
| 20:XT:56:MET:HG3   | 20:XT:84:LEU:HD12  | 1.79                     | 0.64              |
| 25:RA:586:A:H5'    | 29:RF:89:VAL:HG21  | 1.78                     | 0.64              |
| 35:YP:146:VAL:HG22 | 35:YP:147:LEU:H    | 1.62                     | 0.64              |
| 25:YA:320:A:N3     | 29:YF:169:ASN:ND2  | 2.46                     | 0.64              |
| 25:RA:1112:G:OP1   | 31:RH:3:ARG:NH2    | 2.30                     | 0.64              |
| 31:RH:158:HIS:HA   | 31:RH:170:ARG:HG2  | 1.80                     | 0.64              |
| 38:YS:17:ARG:HG3   | 38:YS:17:ARG:HH11  | 1.63                     | 0.64              |
| 9:XI:25:LYS:HD3    | 9:XI:25:LYS:H      | 1.61                     | 0.64              |
| 34:RO:86:ILE:HG22  | 34:RO:94:ARG:HG3   | 1.79                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:QK:124:LYS:NZ   | 11:QK:125:PHE:HE1  | 1.96                     | 0.64              |
| 25:YA:660:G:H21    | 35:YP:12:ALA:HB2   | 1.62                     | 0.64              |
| 25:YA:2439:A:C8    | 25:YA:2439:A:H5'   | 2.33                     | 0.64              |
| 31:RH:51:ARG:HH21  | 31:RH:53:GLU:H     | 1.44                     | 0.64              |
| 1:QA:1177:G:OP2    | 9:QI:97:LYS:NZ     | 2.28                     | 0.64              |
| 25:YA:265:A:N1     | 25:YA:427:U:O2'    | 2.30                     | 0.64              |
| 28:YE:92:THR:OG1   | 28:YE:93:VAL:N     | 2.31                     | 0.64              |
| 41:RV:49:THR:O     | 41:RV:50:PRO:C     | 2.36                     | 0.64              |
| 32:YI:77:LEU:CB    | 32:YI:141:LYS:HB2  | 2.27                     | 0.64              |
| 1:XA:1497:G:C2'    | 1:XA:1498:U:H5'    | 2.28                     | 0.64              |
| 1:QA:1178:G:H5'    | 9:QI:93:ARG:HH21   | 1.62                     | 0.64              |
| 25:RA:642:G:H21    | 25:RA:646:A:H2     | 1.46                     | 0.64              |
| 44:YY:73:ARG:HH21  | 44:YY:82:PRO:HD3   | 1.63                     | 0.64              |
| 1:QA:1158:C:C2'    | 1:QA:1158:C:O2     | 2.34                     | 0.63              |
| 25:YA:2012:G:OP1   | 42:YW:11:ARG:NH2   | 2.26                     | 0.63              |
| 30:YG:114:ILE:HG22 | 30:YG:117:PHE:HB2  | 1.78                     | 0.63              |
| 38:YS:62:LYS:HB3   | 38:YS:97:ARG:HD3   | 1.79                     | 0.63              |
| 26:YB:15:A:H5'     | 26:YB:16:G:C8      | 2.33                     | 0.63              |
| 25:YA:483:A:H5'    | 44:YY:49:VAL:HA    | 1.81                     | 0.63              |
| 25:YA:1930:G:O2'   | 25:YA:1931:U:P     | 2.56                     | 0.63              |
| 30:YG:47:LYS:HD3   | 30:YG:81:LYS:HB2   | 1.80                     | 0.63              |
| 1:XA:951:G:OP2     | 13:XM:102:ARG:NH2  | 2.31                     | 0.63              |
| 4:XD:25:ARG:O      | 4:XD:27:TYR:N      | 2.31                     | 0.63              |
| 25:YA:993:G:OP1    | 40:YU:50:ARG:NH2   | 2.28                     | 0.63              |
| 39:RT:19:LEU:HD22  | 39:RT:86:ILE:HG22  | 1.80                     | 0.63              |
| 32:YI:77:LEU:CD1   | 32:YI:142:VAL:CG2  | 2.72                     | 0.63              |
| 52:Y6:30:THR:CA    | 52:Y6:31:PRO:C     | 2.67                     | 0.63              |
| 22:QW:33:U:H2'     | 22:QW:35:A:OP2     | 1.98                     | 0.63              |
| 31:YH:3:ARG:HH11   | 31:YH:6:ARG:HE     | 1.44                     | 0.63              |
| 25:YA:1300:U:H4'   | 25:YA:1301:A:C5'   | 2.28                     | 0.63              |
| 35:YP:146:VAL:HG22 | 35:YP:147:LEU:HD13 | 1.80                     | 0.63              |
| 50:R4:22:ILE:HG12  | 50:R4:23:GLU:H     | 1.63                     | 0.63              |
| 28:YE:31:CYS:HB3   | 28:YE:49:LEU:HB3   | 1.80                     | 0.63              |
| 21:QU:7:ARG:HG2    | 21:QU:21:TYR:CE1   | 2.34                     | 0.63              |
| 25:RA:247:G:H4'    | 25:RA:386:G:C5     | 2.34                     | 0.63              |
| 25:RA:2384:G:OP2   | 46:R0:55:ARG:NH2   | 2.27                     | 0.63              |
| 25:YA:819:A:OP2    | 25:YA:1187:G:N2    | 2.23                     | 0.63              |
| 1:QA:448:A:OP2     | 1:QA:485:G:N2      | 2.22                     | 0.63              |
| 36:YQ:67:ARG:NH1   | 36:YQ:105:GLU:OE2  | 2.32                     | 0.63              |
| 1:XA:1191:A:H5'    | 3:XC:4:LYS:NZ      | 2.14                     | 0.63              |
| 13:XM:9:ILE:HG13   | 13:XM:10:PRO:CD    | 2.21                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:RH:44:VAL:H     | 31:RH:51:ARG:HH12 | 1.45                     | 0.63              |
| 41:RV:35:LEU:O     | 41:RV:37:VAL:HG22 | 1.99                     | 0.63              |
| 39:RT:125:ARG:O    | 39:RT:129:ARG:NH1 | 2.32                     | 0.63              |
| 16:XP:22:THR:HA    | 16:XP:33:ILE:HG12 | 1.80                     | 0.63              |
| 3:QC:156:ARG:H     | 3:QC:163:ALA:HA   | 1.64                     | 0.63              |
| 25:YA:480:A:H1'    | 44:YY:44:ILE:HD13 | 1.80                     | 0.63              |
| 2:XB:51:LEU:HD23   | 2:XB:201:ILE:HD12 | 1.80                     | 0.63              |
| 25:YA:1400:G:H2'   | 25:YA:1401:G:C8   | 2.34                     | 0.63              |
| 8:QH:42:GLU:HG3    | 8:QH:109:ILE:HD12 | 1.79                     | 0.63              |
| 34:YO:68:GLU:OE2   | 34:YO:78:ARG:NH1  | 2.31                     | 0.63              |
| 10:XJ:46:ARG:HG2   | 10:XJ:64:GLU:HB3  | 1.81                     | 0.63              |
| 31:RH:97:ARG:HB2   | 31:RH:104:GLU:HB2 | 1.79                     | 0.63              |
| 1:QA:1150:U:O4     | 1:QA:1151:A:N6    | 2.31                     | 0.63              |
| 50:Y4:37:SER:OG    | 50:Y4:38:LYS:N    | 2.28                     | 0.63              |
| 25:RA:345:A:O2'    | 25:RA:346:A:N7    | 2.31                     | 0.63              |
| 5:XE:78:HIS:HA     | 8:XH:105:ARG:HG3  | 1.81                     | 0.63              |
| 25:RA:2867:G:HO2'  | 25:RA:2868:A:H8   | 1.44                     | 0.63              |
| 30:YG:67:LYS:H     | 50:Y4:6:HIS:HD2   | 0.84                     | 0.63              |
| 35:RP:60:MET:C     | 35:RP:61:ARG:CG   | 2.63                     | 0.63              |
| 28:RE:47:VAL:HG12  | 28:RE:49:LEU:HD13 | 1.80                     | 0.63              |
| 1:QA:1302:U:H5     | 13:QM:17:VAL:HG21 | 1.63                     | 0.63              |
| 42:RW:68:ARG:NH1   | 42:RW:111:HIS:O   | 2.32                     | 0.63              |
| 50:Y4:61:ARG:HB3   | 50:Y4:62:ARG:HH21 | 1.62                     | 0.63              |
| 38:YS:83:LYS:HE2   | 38:YS:84:GLN:HG3  | 1.80                     | 0.63              |
| 25:YA:1230:C:H2'   | 25:YA:1231:G:H8   | 1.64                     | 0.63              |
| 52:R6:39:TYR:HB3   | 52:R6:41:PRO:HD3  | 1.80                     | 0.63              |
| 29:RF:116:ASP:OD2  | 35:RP:1:MET:N     | 2.32                     | 0.63              |
| 25:RA:643:A:N1     | 25:RA:2369:A:O2'  | 2.31                     | 0.63              |
| 49:R3:11:SER:OG    | 49:R3:13:ILE:HG12 | 1.99                     | 0.63              |
| 45:RZ:156:LYS:HE3  | 45:RZ:156:LYS:N   | 2.14                     | 0.63              |
| 25:RA:993:G:OP1    | 40:RU:50:ARG:NH2  | 2.32                     | 0.63              |
| 52:Y6:28:ARG:CA    | 52:Y6:29:ASN:CB   | 2.77                     | 0.63              |
| 40:RU:90:VAL:HG22  | 41:RV:39:LEU:HB3  | 1.81                     | 0.63              |
| 25:YA:498:G:N3     | 44:YY:47:LYS:NZ   | 2.46                     | 0.63              |
| 25:RA:2822:G:OP1   | 28:RE:159:HIS:NE2 | 2.28                     | 0.63              |
| 36:RQ:37:LEU:HD21  | 36:RQ:130:LYS:HD3 | 1.81                     | 0.63              |
| 45:RZ:119:GLU:OE1  | 45:RZ:122:ARG:NH2 | 2.31                     | 0.63              |
| 9:QI:63:ILE:HG21   | 9:QI:77:ILE:HG12  | 1.81                     | 0.62              |
| 31:YH:125:VAL:HG22 | 31:YH:126:PRO:HA  | 1.81                     | 0.62              |
| 25:YA:1024:G:H3'   | 25:YA:1025:G:H5'' | 1.80                     | 0.62              |
| 1:QA:1006:C:N3     | 1:QA:1023:G:N2    | 2.47                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:QP:71:ARG:HG3   | 16:QP:80:PHE:HE1   | 1.63                     | 0.62              |
| 2:XB:32:ILE:HD11   | 2:XB:40:HIS:HB3    | 1.80                     | 0.62              |
| 25:RA:2200:C:H6    | 25:RA:2200:C:O5'   | 1.81                     | 0.62              |
| 31:RH:84:SER:OG    | 31:RH:85:LYS:N     | 2.32                     | 0.62              |
| 28:RE:78:LEU:HG    | 28:RE:79:ARG:HG2   | 1.79                     | 0.62              |
| 1:XA:1178:G:H5'    | 9:XI:93:ARG:NH2    | 2.14                     | 0.62              |
| 25:RA:1753:G:OP2   | 39:RT:115:ARG:NH2  | 2.33                     | 0.62              |
| 9:QI:103:THR:HG22  | 9:QI:105:ASP:H     | 1.63                     | 0.62              |
| 28:RE:51:PHE:CD1   | 28:RE:52:LEU:HG    | 2.34                     | 0.62              |
| 25:YA:1639:U:H2'   | 25:YA:1640:C:H5''  | 1.81                     | 0.62              |
| 25:RA:1930:G:O2'   | 25:RA:1931:U:P     | 2.57                     | 0.62              |
| 1:QA:1030(C):G:H21 | 1:QA:1030(D):A:H1' | 1.64                     | 0.62              |
| 52:Y6:28:ARG:HB3   | 52:Y6:30:THR:H     | 1.64                     | 0.62              |
| 1:XA:1006:C:N3     | 1:XA:1023:G:N2     | 2.44                     | 0.62              |
| 46:Y0:6:GLY:HA3    | 46:Y0:7:LEU:HD22   | 1.82                     | 0.62              |
| 32:RI:82:ARG:HD2   | 32:RI:146:ALA:HB3  | 1.81                     | 0.62              |
| 50:Y4:40:HIS:H     | 50:Y4:41:PRO:HD2   | 1.64                     | 0.62              |
| 45:YZ:87:ASP:N     | 45:YZ:87:ASP:OD2   | 2.32                     | 0.62              |
| 25:RA:2527:C:H5'   | 55:R9:30:PRO:HB2   | 1.79                     | 0.62              |
| 10:QJ:79:ARG:H     | 10:QJ:79:ARG:HD3   | 1.64                     | 0.62              |
| 27:YD:35:LYS:NZ    | 27:YD:64:ILE:O     | 2.27                     | 0.62              |
| 1:XA:1129:C:H5''   | 9:XI:16:ARG:HH22   | 1.64                     | 0.62              |
| 19:XS:16:LEU:HA    | 19:XS:19:VAL:HG12  | 1.81                     | 0.62              |
| 25:RA:1266:G:O5'   | 42:RW:15:ARG:NH2   | 2.32                     | 0.62              |
| 45:YZ:138:GLU:OE1  | 45:YZ:138:GLU:N    | 2.30                     | 0.62              |
| 9:QI:25:LYS:H      | 9:QI:25:LYS:HD3    | 1.63                     | 0.62              |
| 31:RH:8:PRO:O      | 31:RH:9:ILE:HG12   | 1.97                     | 0.62              |
| 25:RA:2447:G:H4'   | 25:RA:2448:A:C5'   | 2.29                     | 0.62              |
| 2:QB:184:VAL:N     | 2:QB:198:ASP:OD1   | 2.33                     | 0.62              |
| 46:R0:27:GLU:HG3   | 46:R0:68:GLU:HA    | 1.81                     | 0.62              |
| 25:YA:2134:A:N6    | 25:YA:2157:G:O2'   | 2.32                     | 0.62              |
| 25:RA:2208:A:H1'   | 25:RA:2219:G:C4    | 2.35                     | 0.62              |
| 28:RE:49:LEU:HD21  | 28:RE:91:VAL:HG11  | 1.81                     | 0.62              |
| 41:YV:85:LYS:HG3   | 41:YV:87:HIS:N     | 2.13                     | 0.62              |
| 15:QO:56:LEU:HA    | 15:QO:59:MET:HE2   | 1.79                     | 0.62              |
| 4:QD:64:LEU:HD13   | 4:QD:198:VAL:HG21  | 1.81                     | 0.62              |
| 28:YE:70:ALA:O     | 28:YE:72:VAL:N     | 2.32                     | 0.62              |
| 40:RU:76:TYR:OH    | 40:RU:93:LYS:HE2   | 1.98                     | 0.62              |
| 4:QD:23:GLY:O      | 4:QD:24:GLU:HB2    | 1.99                     | 0.62              |
| 1:XA:560:U:H5'     | 1:XA:566:G:N2      | 2.14                     | 0.62              |
| 25:YA:637:A:H5''   | 35:YP:117:GLU:HG3  | 1.81                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1548:C:N3    | 25:RA:1549:C:C5    | 2.68                     | 0.62              |
| 1:XA:1379:G:O6     | 7:XG:3:ARG:HD3     | 2.00                     | 0.62              |
| 19:XS:36:ARG:NH1   | 19:XS:73:GLU:HB2   | 2.14                     | 0.62              |
| 9:QI:17:VAL:HG11   | 9:QI:81:ILE:HA     | 1.81                     | 0.62              |
| 25:YA:2134:A:OP2   | 25:YA:2157:G:N2    | 2.33                     | 0.62              |
| 6:QF:28:ARG:NH2    | 6:QF:31:GLU:OE1    | 2.33                     | 0.62              |
| 26:YB:8:U:O3'      | 38:YS:25:ARG:NH2   | 2.32                     | 0.62              |
| 39:YT:105:LEU:HD22 | 39:YT:109:GLU:HG3  | 1.80                     | 0.62              |
| 45:YZ:19:ARG:NH1   | 45:YZ:84:GLU:O     | 2.33                     | 0.62              |
| 9:QI:8:GLY:HA2     | 9:QI:79:LEU:HD12   | 1.82                     | 0.62              |
| 25:RA:2445:G:OP1   | 29:RF:74:ARG:NH2   | 2.31                     | 0.62              |
| 31:RH:42:ARG:O     | 31:RH:51:ARG:NH2   | 2.32                     | 0.62              |
| 13:XM:2:ALA:O      | 13:XM:4:ILE:N      | 2.32                     | 0.62              |
| 29:RF:157:VAL:HB   | 29:RF:194:MET:HB3  | 1.82                     | 0.62              |
| 25:RA:2564:A:C2    | 25:RA:2647:U:H4'   | 2.35                     | 0.62              |
| 15:XO:82:ILE:HD11  | 15:XO:88:ARG:HB2   | 1.81                     | 0.62              |
| 25:RA:1007:C:OP1   | 33:RN:35:ARG:NH1   | 2.32                     | 0.62              |
| 9:QI:17:VAL:HG22   | 9:QI:63:ILE:HG12   | 1.81                     | 0.62              |
| 52:R6:9:LEU:HB3    | 52:R6:27:LYS:HA    | 1.82                     | 0.62              |
| 5:QE:102:ALA:HB1   | 5:QE:106:PRO:HG2   | 1.81                     | 0.62              |
| 25:YA:1056:G:H4'   | 25:YA:1086:A:H1'   | 1.82                     | 0.62              |
| 25:YA:686:G:H21    | 25:YA:788:A:H61    | 1.47                     | 0.62              |
| 9:QI:96:LEU:HD23   | 9:QI:102:LEU:HD12  | 1.81                     | 0.62              |
| 45:YZ:150:LEU:HD21 | 45:YZ:155:LEU:HD23 | 1.80                     | 0.62              |
| 23:QX:12:A:H2'     | 23:QX:13:A:C8      | 2.35                     | 0.62              |
| 1:QA:1347:G:H1'    | 1:QA:1348:U:OP2    | 2.00                     | 0.62              |
| 1:XA:17:U:H2'      | 1:XA:18:C:C6       | 2.35                     | 0.62              |
| 2:XB:24:TRP:HD1    | 2:XB:24:TRP:H      | 1.46                     | 0.62              |
| 1:QA:1297:C:O2'    | 7:QG:114:ARG:NH2   | 2.33                     | 0.62              |
| 10:QJ:34:VAL:HG22  | 10:QJ:74:ILE:HG22  | 1.80                     | 0.62              |
| 31:YH:51:ARG:HH21  | 31:YH:53:GLU:H     | 1.48                     | 0.61              |
| 1:XA:422:C:HO2'    | 1:XA:423:G:N2      | 1.97                     | 0.61              |
| 1:XA:1152:A:H5''   | 10:XJ:13:HIS:CD2   | 2.34                     | 0.61              |
| 25:YA:1322:A:N1    | 25:YA:1333:C:O2'   | 2.29                     | 0.61              |
| 1:XA:1126:U:H3     | 10:XJ:40:LEU:HD21  | 1.63                     | 0.61              |
| 9:QI:4:TYR:HB2     | 9:QI:18:PHE:O      | 2.00                     | 0.61              |
| 45:RZ:118:GLN:HG3  | 45:RZ:173:ALA:N    | 2.14                     | 0.61              |
| 1:XA:1314:C:H2'    | 1:XA:1315:U:C6     | 2.35                     | 0.61              |
| 25:RA:2875:C:H4'   | 39:RT:5:ALA:HB2    | 1.82                     | 0.61              |
| 35:RP:62:LEU:HD12  | 54:R8:25:MET:HB3   | 1.82                     | 0.61              |
| 25:RA:2848:G:O2'   | 25:RA:2867:G:N2    | 2.33                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:Y4:66:SER:HA   | 50:Y4:68:ARG:HH11 | 1.65                     | 0.61              |
| 25:RA:1329:U:H5'' | 25:RA:1330:C:H5   | 1.65                     | 0.61              |
| 29:RF:132:VAL:O   | 29:RF:134:GLY:N   | 2.30                     | 0.61              |
| 10:XJ:49:VAL:HG13 | 14:XN:41:ARG:CD   | 2.27                     | 0.61              |
| 2:XB:47:THR:HA    | 2:XB:202:PRO:HG2  | 1.81                     | 0.61              |
| 1:QA:1352:C:OP1   | 21:QU:3:LYS:NZ    | 2.28                     | 0.61              |
| 1:QA:728:A:H2'    | 1:QA:729:A:C8     | 2.33                     | 0.61              |
| 19:QS:50:ALA:HB1  | 19:QS:57:HIS:HB3  | 1.82                     | 0.61              |
| 3:QC:153:VAL:HG22 | 3:QC:198:VAL:HG22 | 1.82                     | 0.61              |
| 25:YA:1112:G:OP1  | 31:YH:3:ARG:NH2   | 2.33                     | 0.61              |
| 25:RA:1021:A:H3'  | 25:RA:1021:A:C8   | 2.35                     | 0.61              |
| 27:RD:35:LYS:HG2  | 27:RD:64:ILE:N    | 2.15                     | 0.61              |
| 1:XA:974:A:OP1    | 14:XN:29:ARG:NH2  | 2.33                     | 0.61              |
| 8:XH:33:GLU:OE1   | 8:XH:50:ARG:NH1   | 2.34                     | 0.61              |
| 32:RI:31:LEU:HD21 | 32:RI:38:LEU:HG   | 1.82                     | 0.61              |
| 25:YA:1907:G:O2'  | 25:YA:1908:C:H5'  | 2.00                     | 0.61              |
| 31:RH:10:PRO:C    | 31:RH:11:VAL:HG12 | 2.21                     | 0.61              |
| 23:QX:13:A:O2'    | 23:QX:14:A:H5''   | 2.00                     | 0.61              |
| 25:RA:2232:U:P    | 47:R1:40:ARG:HH12 | 2.22                     | 0.61              |
| 54:Y8:8:LYS:HB3   | 54:Y8:12:LYS:HE3  | 1.83                     | 0.61              |
| 1:QA:422:C:O2'    | 1:QA:423:G:N2     | 2.34                     | 0.61              |
| 1:QA:354:G:N1     | 1:QA:355:C:C4     | 2.69                     | 0.61              |
| 31:YH:26:VAL:HG11 | 31:YH:75:ALA:HB1  | 1.83                     | 0.61              |
| 2:QB:29:ALA:HB1   | 2:QB:30:ARG:HH21  | 1.65                     | 0.61              |
| 52:Y6:15:GLU:OE1  | 52:Y6:44:ARG:NH2  | 2.28                     | 0.61              |
| 23:XX:14:A:O2'    | 23:XX:15:A:H5'    | 2.01                     | 0.61              |
| 1:QA:973:G:OP1    | 10:QJ:57:LYS:NZ   | 2.33                     | 0.61              |
| 1:QA:1152:A:H5''  | 10:QJ:13:HIS:CD2  | 2.36                     | 0.61              |
| 25:YA:907:U:OP1   | 36:YQ:24:GLY:N    | 2.31                     | 0.61              |
| 48:R2:15:LYS:HA   | 48:R2:67:LYS:HZ1  | 1.65                     | 0.61              |
| 29:YF:79:GLY:HA2  | 29:YF:86:GLY:HA2  | 1.82                     | 0.61              |
| 1:QA:1123:A:H4'   | 10:QJ:37:PRO:HD2  | 1.82                     | 0.61              |
| 25:YA:747:U:OP2   | 51:Y5:3:LYS:HD3   | 2.00                     | 0.61              |
| 52:Y6:34:LEU:H    | 52:Y6:34:LEU:HD23 | 1.65                     | 0.61              |
| 25:YA:832:G:H5'   | 35:YP:45:LEU:HD21 | 1.81                     | 0.61              |
| 1:QA:1289:A:OP1   | 21:QU:9:ARG:NH2   | 2.33                     | 0.61              |
| 21:XU:25:LYS:HG2  | 21:XU:26:LYS:HG2  | 1.82                     | 0.61              |
| 7:XG:113:GLU:HB2  | 7:XG:119:ARG:HG2  | 1.83                     | 0.61              |
| 25:YA:969:U:H2'   | 25:YA:970:C:C6    | 2.36                     | 0.61              |
| 8:XH:25:ASP:N     | 8:XH:25:ASP:OD1   | 2.33                     | 0.61              |
| 8:QH:110:ALA:HB3  | 8:QH:121:ASP:HB3  | 1.81                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:128:C:H2'   | 25:RA:129:C:C6     | 2.36                     | 0.61              |
| 27:RD:44:ASN:HB3  | 27:RD:49:ILE:HA    | 1.82                     | 0.61              |
| 1:QA:436:C:H2'    | 1:QA:437:U:H6      | 1.66                     | 0.61              |
| 49:R3:6:VAL:HG22  | 49:R3:56:VAL:HG23  | 1.83                     | 0.61              |
| 31:RH:18:GLU:HB2  | 31:RH:25:LYS:HB2   | 1.83                     | 0.61              |
| 34:YO:92:GLU:OE1  | 34:YO:113:LYS:NZ   | 2.33                     | 0.61              |
| 24:QY:90:ASP:OD1  | 24:QY:91:TYR:N     | 2.33                     | 0.61              |
| 1:QA:350:G:C8     | 1:QA:350:G:C5'     | 2.84                     | 0.60              |
| 25:RA:686:G:H5''  | 53:R7:11:LYS:HE2   | 1.83                     | 0.60              |
| 2:QB:55:PHE:HD1   | 2:QB:221:LEU:HD21  | 1.66                     | 0.60              |
| 50:R4:40:HIS:H    | 50:R4:41:PRO:HD2   | 1.66                     | 0.60              |
| 25:RA:2472:G:N1   | 25:RA:2477:C:OP1   | 2.28                     | 0.60              |
| 1:XA:814:A:H2'    | 1:XA:816:A:H5''    | 1.83                     | 0.60              |
| 25:RA:654(D):G:H1 | 25:RA:654(Q):C:H42 | 1.47                     | 0.60              |
| 1:QA:1305:G:H22   | 1:QA:1331:G:H2'    | 1.65                     | 0.60              |
| 13:XM:10:PRO:HG2  | 13:XM:18:ALA:CB    | 2.31                     | 0.60              |
| 25:RA:764:A:N3    | 27:RD:213:ARG:NH1  | 2.49                     | 0.60              |
| 2:QB:24:TRP:HD1   | 2:QB:24:TRP:H      | 1.48                     | 0.60              |
| 4:QD:107:ARG:HH21 | 4:QD:194:LEU:HD12  | 1.66                     | 0.60              |
| 22:QV:54:U:O2'    | 22:QV:55:U:H5'     | 2.00                     | 0.60              |
| 12:QL:88:GLY:H    | 12:QL:98:TYR:HA    | 1.65                     | 0.60              |
| 25:RA:1862:G:H1   | 25:RA:1880:C:H42   | 1.48                     | 0.60              |
| 1:QA:1379:G:C8    | 7:QG:3:ARG:HD3     | 2.36                     | 0.60              |
| 1:XA:1435:G:H2'   | 1:XA:1436:U:C6     | 2.36                     | 0.60              |
| 2:QB:32:ILE:HD11  | 2:QB:40:HIS:HB3    | 1.82                     | 0.60              |
| 1:QA:662:G:H2'    | 1:QA:663:A:C8      | 2.36                     | 0.60              |
| 2:QB:47:THR:HA    | 2:QB:202:PRO:HG2   | 1.83                     | 0.60              |
| 25:YA:655:A:H4'   | 25:YA:656:G:H5'    | 1.83                     | 0.60              |
| 3:QC:60:ALA:O     | 3:QC:63:ASN:ND2    | 2.34                     | 0.60              |
| 49:R3:8:LEU:HD13  | 49:R3:31:LEU:HD12  | 1.82                     | 0.60              |
| 25:RA:2685:G:H1'  | 25:RA:2726:U:H5    | 1.66                     | 0.60              |
| 52:R6:33:LYS:HD2  | 52:R6:34:LEU:H     | 1.66                     | 0.60              |
| 4:XD:127:THR:HA   | 4:XD:132:ARG:HA    | 1.83                     | 0.60              |
| 44:YY:76:CYS:O    | 44:YY:77:PRO:C     | 2.39                     | 0.60              |
| 1:XA:677:U:H2'    | 1:XA:678:U:H6      | 1.66                     | 0.60              |
| 19:XS:9:VAL:HG11  | 50:Y4:63:TYR:HB2   | 1.83                     | 0.60              |
| 25:RA:583:G:OP2   | 40:RU:10:ARG:NH1   | 2.31                     | 0.60              |
| 27:YD:95:LEU:HD11 | 27:YD:105:ILE:HG23 | 1.82                     | 0.60              |
| 41:RV:69:LYS:HD2  | 41:RV:85:LYS:HD2   | 1.82                     | 0.60              |
| 1:QA:350:G:H5'    | 1:QA:350:G:H8      | 1.65                     | 0.60              |
| 41:RV:71:LEU:N    | 41:RV:86:GLY:HA3   | 2.16                     | 0.60              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:YA:2404:C:H1'   | 35:YP:67:MET:CE     | 2.32                     | 0.60              |
| 44:RY:13:VAL:HG23  | 44:RY:73:ARG:O      | 2.00                     | 0.60              |
| 27:RD:35:LYS:HG2   | 27:RD:64:ILE:H      | 1.67                     | 0.60              |
| 21:XU:12:LYS:HB3   | 21:XU:22:ARG:HD2    | 1.83                     | 0.60              |
| 25:RA:1418:G:OP1   | 25:RA:1588:C:O2'    | 2.20                     | 0.60              |
| 32:RI:4:ILE:HG12   | 32:RI:18:VAL:HG22   | 1.82                     | 0.60              |
| 32:RI:143:SER:O    | 32:RI:144:VAL:HG12  | 2.02                     | 0.60              |
| 25:RA:1695:G:H2'   | 25:RA:1696:G:C5'    | 2.32                     | 0.60              |
| 25:YA:2646:C:H2'   | 25:YA:2647:U:O4'    | 2.02                     | 0.60              |
| 25:RA:1918:A:O2'   | 25:RA:1920:C:N4     | 2.35                     | 0.60              |
| 25:YA:686:G:N2     | 25:YA:788:A:H61     | 2.00                     | 0.60              |
| 27:RD:35:LYS:HD2   | 27:RD:104:TYR:CE1   | 2.37                     | 0.60              |
| 32:YI:131:LYS:HB3  | 32:YI:132:PRO:HA    | 1.84                     | 0.60              |
| 20:XT:75:ASN:OD1   | 20:XT:75:ASN:N      | 2.31                     | 0.60              |
| 1:XA:1380:U:C4     | 7:XG:2:ALA:HA       | 2.36                     | 0.60              |
| 25:YA:2016:U:O4'   | 51:Y5:6:VAL:HG11    | 2.02                     | 0.60              |
| 27:RD:108:PRO:HG2  | 27:RD:111:LEU:HB2   | 1.83                     | 0.60              |
| 18:QR:22:VAL:HG12  | 18:QR:56:THR:HA     | 1.82                     | 0.60              |
| 28:RE:67:PHE:O     | 28:RE:69:LYS:N      | 2.33                     | 0.60              |
| 25:YA:956:G:OP2    | 36:YQ:14:ARG:NH2    | 2.35                     | 0.60              |
| 25:RA:614(A):U:O2' | 25:RA:614(B):G:H5'  | 2.01                     | 0.60              |
| 25:YA:1454:U:OP1   | 37:YR:77:ARG:NH1    | 2.34                     | 0.60              |
| 29:RF:1:MET:O      | 29:RF:2:LYS:O       | 2.20                     | 0.60              |
| 27:YD:17:THR:O     | 27:YD:211:ARG:NH2   | 2.35                     | 0.60              |
| 25:RA:2583:G:H2'   | 25:RA:2584:U:H5'    | 1.82                     | 0.60              |
| 1:XA:957:U:H2'     | 1:XA:959:A:OP2      | 2.02                     | 0.60              |
| 12:QL:23:LYS:HD3   | 12:QL:23:LYS:H      | 1.67                     | 0.60              |
| 9:XI:110:GLU:OE2   | 9:XI:113:LYS:NZ     | 2.33                     | 0.60              |
| 1:XA:1060:C:H3'    | 3:XC:3:ASN:ND2      | 2.16                     | 0.60              |
| 54:R8:29:LYS:O     | 54:R8:31:HIS:N      | 2.35                     | 0.60              |
| 25:RA:857:C:H1'    | 46:R0:26:TYR:HE2    | 1.66                     | 0.60              |
| 26:YB:51:G:N7      | 38:YS:62:LYS:NZ     | 2.44                     | 0.60              |
| 45:RZ:157:LEU:N    | 45:RZ:158:PRO:HD3   | 2.17                     | 0.59              |
| 1:QA:1442(A):G:H3' | 1:QA:1442(B):A:H5'' | 1.84                     | 0.59              |
| 13:XM:99:ARG:HD3   | 13:XM:101:GLN:HG3   | 1.84                     | 0.59              |
| 5:XE:137:GLU:OE1   | 5:XE:141:GLN:NE2    | 2.35                     | 0.59              |
| 1:QA:1227:A:C4     | 13:QM:117:VAL:HG21  | 2.37                     | 0.59              |
| 2:QB:87:ARG:HH21   | 2:QB:233:SER:HB2    | 1.67                     | 0.59              |
| 52:R6:11:LEU:HD12  | 52:R6:53:LYS:HB3    | 1.83                     | 0.59              |
| 25:RA:141:A:H8     | 25:RA:1408:C:HO2'   | 1.48                     | 0.59              |
| 1:QA:677:U:H3      | 1:QA:713:G:H22      | 1.47                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:2466:C:H5'' | 55:R9:6:SER:HB2    | 1.83                     | 0.59              |
| 44:RY:42:VAL:HG13 | 44:RY:65:ALA:HB3   | 1.83                     | 0.59              |
| 2:XB:25:ASN:O     | 2:XB:27:LYS:N      | 2.34                     | 0.59              |
| 27:YD:237:GLU:O   | 27:YD:239:ARG:N    | 2.36                     | 0.59              |
| 1:QA:717:C:H4'    | 11:QK:117:ASN:CB   | 2.32                     | 0.59              |
| 25:RA:873:G:H1    | 25:RA:904:C:H42    | 1.49                     | 0.59              |
| 10:XJ:61:GLU:OE2  | 14:XN:45:ARG:NH1   | 2.35                     | 0.59              |
| 44:RY:14:LEU:HA   | 44:RY:24:VAL:HA    | 1.83                     | 0.59              |
| 39:YT:118:ARG:HA  | 39:YT:121:ILE:HB   | 1.83                     | 0.59              |
| 31:YH:152:ARG:HG3 | 31:YH:153:LYS:HG2  | 1.83                     | 0.59              |
| 19:XS:48:THR:HG22 | 19:XS:61:TYR:HD1   | 1.67                     | 0.59              |
| 39:RT:27:THR:HG23 | 39:RT:90:GLN:HB3   | 1.84                     | 0.59              |
| 1:XA:1105:A:H2'   | 1:XA:1106:G:H8     | 1.67                     | 0.59              |
| 10:XJ:49:VAL:CG1  | 14:XN:41:ARG:HD2   | 2.26                     | 0.59              |
| 25:YA:298:G:OP1   | 44:YY:84:ARG:O     | 2.20                     | 0.59              |
| 28:YE:63:LEU:HG   | 28:YE:64:LYS:N     | 2.16                     | 0.59              |
| 25:RA:1548:C:N3   | 25:RA:1549:C:C4    | 2.70                     | 0.59              |
| 22:QW:19:G:C6     | 25:RA:2112:G:N2    | 2.70                     | 0.59              |
| 52:Y6:14:THR:OG1  | 52:Y6:15:GLU:N     | 2.34                     | 0.59              |
| 2:QB:132:LYS:O    | 2:QB:134:GLU:N     | 2.35                     | 0.59              |
| 4:QD:111:ALA:HB2  | 4:QD:120:LEU:HD12  | 1.84                     | 0.59              |
| 25:RA:2096:U:H3   | 25:RA:2193:G:H1    | 1.50                     | 0.59              |
| 25:YA:2401:U:H5'  | 52:Y6:18:ARG:HH12  | 1.67                     | 0.59              |
| 29:YF:116:ASP:OD2 | 35:YP:1:MET:N      | 2.36                     | 0.59              |
| 28:YE:111:ARG:HA  | 37:YR:2:ARG:NH1    | 2.16                     | 0.59              |
| 25:RA:2010:G:H5'' | 42:RW:42:ARG:HB2   | 1.82                     | 0.59              |
| 7:XG:73:MET:HG2   | 7:XG:90:GLU:HA     | 1.84                     | 0.59              |
| 42:RW:19:LEU:HB3  | 51:R5:25:LEU:HD12  | 1.85                     | 0.59              |
| 1:XA:1379:G:O6    | 7:XG:3:ARG:CD      | 2.50                     | 0.59              |
| 35:YP:9:ASN:N     | 35:YP:9:ASN:OD1    | 2.32                     | 0.59              |
| 1:QA:345:C:O2'    | 1:QA:346:G:O5'     | 2.21                     | 0.59              |
| 25:YA:1932:A:H2'  | 25:YA:1933:G:O4'   | 2.01                     | 0.59              |
| 25:RA:1266:G:OP2  | 51:R5:19:ARG:NH1   | 2.35                     | 0.59              |
| 1:XA:544:G:OP1    | 4:XD:59:ARG:NH2    | 2.27                     | 0.59              |
| 2:XB:115:LEU:HD13 | 2:XB:145:LEU:HB3   | 1.85                     | 0.59              |
| 25:RA:2093:G:N2   | 25:RA:2197:U:C2    | 2.70                     | 0.59              |
| 35:YP:83:VAL:HG12 | 35:YP:112:LEU:HD21 | 1.84                     | 0.59              |
| 1:XA:7:G:H5'      | 1:XA:298:A:O4'     | 2.02                     | 0.59              |
| 34:YO:35:VAL:HG11 | 34:YO:103:ALA:HB3  | 1.82                     | 0.59              |
| 25:RA:1548:C:N4   | 25:RA:1549:C:H41   | 2.00                     | 0.59              |
| 39:YT:106:SER:HA  | 39:YT:110:ILE:HG13 | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:QG:5:ARG:HH21   | 7:QG:7:ALA:HA     | 1.67                     | 0.59              |
| 46:Y0:27:GLU:HG3  | 46:Y0:68:GLU:HA   | 1.84                     | 0.59              |
| 1:XA:345:C:OP2    | 39:YT:39:ARG:NH2  | 2.35                     | 0.59              |
| 3:QC:108:ASN:HD21 | 3:QC:144:SER:HB2  | 1.68                     | 0.59              |
| 1:QA:1347:G:C8    | 9:QI:107:ARG:HB3  | 2.38                     | 0.59              |
| 1:XA:1151:A:H2'   | 1:XA:1152:A:C8    | 2.37                     | 0.59              |
| 29:YF:143:ALA:HB1 | 29:YF:148:LEU:HB2 | 1.84                     | 0.59              |
| 3:XC:150:LYS:HE2  | 3:XC:152:ILE:HD11 | 1.84                     | 0.59              |
| 1:XA:1158:C:C4    | 1:XA:1160:G:C8    | 2.91                     | 0.59              |
| 25:RA:2786:U:O2   | 28:RE:62:PRO:HB3  | 2.03                     | 0.59              |
| 29:YF:132:VAL:O   | 29:YF:134:GLY:N   | 2.34                     | 0.59              |
| 16:XP:11:SER:HB2  | 16:XP:14:ASN:HB3  | 1.84                     | 0.59              |
| 26:YB:11:C:OP2    | 46:Y0:72:ARG:NH1  | 2.35                     | 0.59              |
| 30:YG:129:GLY:HA2 | 30:YG:166:ASP:HA  | 1.85                     | 0.59              |
| 55:Y9:8:LYS:O     | 55:Y9:34:GLN:NE2  | 2.35                     | 0.59              |
| 1:XA:1061:G:OP2   | 3:XC:3:ASN:ND2    | 2.31                     | 0.59              |
| 25:YA:67:U:N3     | 25:YA:74:A:C2     | 2.71                     | 0.59              |
| 27:YD:35:LYS:HB3  | 27:YD:63:ARG:HA   | 1.83                     | 0.59              |
| 1:XA:1306:A:N6    | 1:XA:1331:G:O2'   | 2.36                     | 0.59              |
| 52:Y6:13:CYS:H    | 52:Y6:22:ALA:HB3  | 1.67                     | 0.59              |
| 31:RH:44:VAL:HG22 | 31:RH:51:ARG:HH11 | 1.68                     | 0.59              |
| 31:RH:44:VAL:H    | 31:RH:51:ARG:NH1  | 2.01                     | 0.59              |
| 15:XO:87:ILE:HG22 | 15:XO:88:ARG:H    | 1.67                     | 0.59              |
| 25:RA:185:U:H4'   | 25:RA:218:A:H4'   | 1.85                     | 0.59              |
| 39:RT:24:PRO:HA   | 39:RT:49:VAL:HG13 | 1.84                     | 0.59              |
| 25:YA:142:G:H4'   | 43:YX:35:THR:HG21 | 1.84                     | 0.59              |
| 48:Y2:41:ILE:HD11 | 48:Y2:44:LEU:HD12 | 1.85                     | 0.59              |
| 28:YE:37:ARG:HD3  | 28:YE:44:TYR:OH   | 2.03                     | 0.59              |
| 35:YP:128:HIS:O   | 35:YP:147:LEU:HB3 | 2.03                     | 0.59              |
| 19:XS:45:VAL:HG13 | 19:XS:62:ILE:HG22 | 1.85                     | 0.59              |
| 19:XS:5:LEU:HD13  | 19:XS:9:VAL:HA    | 1.83                     | 0.59              |
| 1:QA:148:G:H2'    | 1:QA:149:A:H8     | 1.68                     | 0.59              |
| 1:QA:675:A:H1'    | 11:QK:116:HIS:CE1 | 2.38                     | 0.58              |
| 25:YA:2010:G:C6   | 25:YA:2011:U:C4   | 2.91                     | 0.58              |
| 11:XK:54:ARG:NH1  | 11:XK:54:ARG:HG2  | 2.17                     | 0.58              |
| 42:RW:59:VAL:HG23 | 42:RW:65:LEU:H    | 1.68                     | 0.58              |
| 1:XA:1513:A:H2'   | 1:XA:1514:C:C6    | 2.37                     | 0.58              |
| 25:YA:2692:C:H2'  | 25:YA:2693:A:H8   | 1.68                     | 0.58              |
| 35:RP:26:GLY:O    | 35:RP:28:GLY:N    | 2.35                     | 0.58              |
| 45:RZ:125:LEU:HG  | 45:RZ:164:ALA:HB3 | 1.84                     | 0.58              |
| 43:RX:63:LYS:HZ2  | 43:RX:63:LYS:H    | 1.51                     | 0.58              |

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| Atom-1               | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-------------------|--------------------------|-------------------|
| 25:RA:2776:A:OP1     | 25:RA:2776:A:H3'  | 2.03                     | 0.58              |
| 44:YY:33:LYS:HD3     | 44:YY:33:LYS:H    | 1.68                     | 0.58              |
| 20:QT:53:LEU:HB3     | 20:QT:102:GLY:HA3 | 1.85                     | 0.58              |
| 1:XA:677:U:H2'       | 1:XA:678:U:C6     | 2.38                     | 0.58              |
| 22:XW:58:A:H1'       | 22:XW:60:U:C5     | 2.38                     | 0.58              |
| 45:YZ:27:VAL:HG13    | 45:YZ:87:ASP:HB3  | 1.84                     | 0.58              |
| 1:QA:309:G:O2'       | 1:QA:607:A:N1     | 2.35                     | 0.58              |
| 25:RA:2712(A):A:H5'' | 25:RA:2713:A:OP2  | 2.03                     | 0.58              |
| 13:XM:86:CYS:HB2     | 19:XS:73:GLU:HB3  | 1.85                     | 0.58              |
| 29:RF:2:LYS:HB2      | 29:RF:24:LEU:HD12 | 1.83                     | 0.58              |
| 1:QA:349:A:H3'       | 1:QA:350:G:H5''   | 1.83                     | 0.58              |
| 9:QI:28:VAL:HG11     | 9:QI:63:ILE:H     | 1.67                     | 0.58              |
| 25:RA:530:G:N1       | 25:RA:2023:G:OP1  | 2.31                     | 0.58              |
| 25:RA:2415:G:H4'     | 35:RP:67:MET:N    | 2.19                     | 0.58              |
| 25:RA:709:U:H2'      | 25:RA:710:G:C8    | 2.39                     | 0.58              |
| 45:YZ:5:LEU:HB3      | 45:YZ:59:LEU:HA   | 1.85                     | 0.58              |
| 25:YA:6:A:C2         | 25:YA:7:G:N9      | 2.71                     | 0.58              |
| 51:R5:4:HIS:HB3      | 51:R5:5:PRO:CD    | 2.31                     | 0.58              |
| 41:YV:2:PHE:CD2      | 41:YV:42:GLY:HA2  | 2.38                     | 0.58              |
| 1:XA:1125:U:H2'      | 1:XA:1126:U:H2'   | 1.85                     | 0.58              |
| 36:RQ:80:GLU:HG3     | 46:R0:5:LYS:HB3   | 1.84                     | 0.58              |
| 1:XA:1229:A:OP2      | 13:XM:114:ARG:HD3 | 2.03                     | 0.58              |
| 1:QA:8:A:N6          | 4:QD:205:GLU:O    | 2.36                     | 0.58              |
| 25:RA:1227:G:OP2     | 40:RU:16:LYS:NZ   | 2.28                     | 0.58              |
| 25:RA:882:G:H1       | 25:RA:894:C:H42   | 1.51                     | 0.58              |
| 1:QA:666:G:H5'       | 1:QA:726:C:H1'    | 1.85                     | 0.58              |
| 1:XA:1493:A:H1'      | 24:XY:55:PRO:HD3  | 1.86                     | 0.58              |
| 19:QS:65:ASN:HA      | 50:R4:55:ARG:HD2  | 1.86                     | 0.58              |
| 50:Y4:55:ARG:HE      | 50:Y4:56:VAL:H    | 1.51                     | 0.58              |
| 25:YA:747:U:C5       | 51:Y5:3:LYS:HB2   | 2.39                     | 0.58              |
| 13:XM:23:TYR:HB3     | 13:XM:67:GLU:HA   | 1.85                     | 0.58              |
| 25:RA:2823:A:OP1     | 28:RE:113:PHE:HB2 | 2.03                     | 0.58              |
| 1:XA:1322:C:H5''     | 13:XM:100:GLY:HA3 | 1.84                     | 0.58              |
| 25:RA:942:G:OP2      | 35:RP:39:LYS:NZ   | 2.36                     | 0.58              |
| 50:R4:66:SER:HA      | 50:R4:68:ARG:HH11 | 1.68                     | 0.58              |
| 6:XF:70:ASP:OD1      | 6:XF:70:ASP:N     | 2.37                     | 0.58              |
| 27:YD:148:GLU:HB2    | 27:YD:151:LYS:HD2 | 1.86                     | 0.58              |
| 44:YY:79:CYS:O       | 44:YY:80:GLY:O    | 2.21                     | 0.58              |
| 44:RY:76:CYS:HB3     | 44:RY:96:ILE:HD11 | 1.86                     | 0.58              |
| 28:YE:60:ASN:HB3     | 28:YE:62:PRO:HD2  | 1.84                     | 0.58              |
| 9:QI:10:ARG:NH2      | 9:QI:11:LYS:HD3   | 2.14                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:1695:G:H2'   | 25:RA:1696:G:O4'   | 2.03                     | 0.58              |
| 35:RP:55:ARG:HG2   | 35:RP:56:SER:N     | 2.18                     | 0.58              |
| 2:QB:32:ILE:HG12   | 2:QB:33:TYR:H      | 1.67                     | 0.58              |
| 26:RB:56:G:H5'     | 30:RG:27:ASN:HD21  | 1.68                     | 0.58              |
| 25:YA:1482:U:H5'   | 25:YA:1483:G:OP2   | 2.03                     | 0.58              |
| 7:XG:20:ASP:OD2    | 7:XG:23:VAL:N      | 2.35                     | 0.58              |
| 25:YA:2830:G:H5'   | 28:YE:58:ARG:HH11  | 1.69                     | 0.58              |
| 44:RY:47:LYS:HA    | 44:RY:60:PHE:HB3   | 1.84                     | 0.58              |
| 6:QF:83:ASP:OD2    | 6:QF:83:ASP:N      | 2.36                     | 0.58              |
| 9:XI:2:GLU:O       | 9:XI:20:ARG:NH1    | 2.37                     | 0.58              |
| 28:YE:95:ILE:H     | 28:YE:95:ILE:HD12  | 1.68                     | 0.58              |
| 35:RP:62:LEU:CD1   | 54:R8:25:MET:HB3   | 2.34                     | 0.58              |
| 1:XA:1227:A:C4     | 13:XM:117:VAL:HG21 | 2.38                     | 0.58              |
| 25:RA:2092:U:OP1   | 25:RA:2199:A:O2'   | 2.22                     | 0.58              |
| 2:XB:14:GLY:O      | 2:XB:209:ARG:NH1   | 2.35                     | 0.58              |
| 25:YA:1614:A:H62   | 42:YW:93:ALA:HB2   | 1.68                     | 0.58              |
| 28:YE:132:HIS:O    | 28:YE:134:ILE:HG23 | 2.03                     | 0.58              |
| 27:RD:169:GLU:HG2  | 27:RD:174:ILE:HD11 | 1.85                     | 0.58              |
| 52:Y6:28:ARG:HB3   | 52:Y6:30:THR:N     | 2.18                     | 0.58              |
| 28:RE:11:MET:HA    | 28:RE:24:THR:HA    | 1.86                     | 0.58              |
| 13:QM:97:PRO:HA    | 13:QM:110:ARG:HD3  | 1.86                     | 0.58              |
| 28:YE:52:LEU:O     | 28:YE:74:PRO:HA    | 2.04                     | 0.58              |
| 19:QS:67:VAL:HG11  | 50:R4:55:ARG:HB2   | 1.86                     | 0.58              |
| 25:YA:620:G:H5'    | 25:YA:620:G:N3     | 2.19                     | 0.58              |
| 52:R6:42:TRP:HD1   | 52:R6:44:ARG:HG2   | 1.69                     | 0.58              |
| 19:XS:72:GLY:HA2   | 19:XS:75:ALA:HB3   | 1.86                     | 0.58              |
| 21:QU:6:ARG:CZ     | 21:QU:15:ARG:HH21  | 2.17                     | 0.58              |
| 25:RA:463:G:N2     | 25:RA:466:A:OP2    | 2.34                     | 0.58              |
| 13:XM:19:LEU:HB3   | 13:XM:25:ILE:HG21  | 1.86                     | 0.58              |
| 2:XB:55:PHE:HD1    | 2:XB:221:LEU:HD21  | 1.68                     | 0.58              |
| 30:YG:67:LYS:HD2   | 50:Y4:5:ILE:HG12   | 1.86                     | 0.58              |
| 42:RW:88:ARG:HB3   | 42:RW:92:ARG:HB3   | 1.86                     | 0.58              |
| 52:Y6:10:LEU:HA    | 52:Y6:24:GLU:OE1   | 2.04                     | 0.58              |
| 25:YA:637:A:O5'    | 35:YP:116:GLY:HA2  | 2.04                     | 0.58              |
| 29:RF:132:VAL:HG22 | 29:RF:133:ASN:H    | 1.69                     | 0.58              |
| 25:RA:559:G:H22    | 40:RU:49:HIS:CE1   | 2.22                     | 0.58              |
| 45:YZ:165:VAL:HG22 | 45:YZ:166:SER:H    | 1.68                     | 0.58              |
| 1:XA:1123:A:H4'    | 10:XJ:36:GLY:HA3   | 1.86                     | 0.58              |
| 25:YA:1174:A:H62   | 25:YA:1177:A:H4'   | 1.69                     | 0.58              |
| 8:XH:41:ARG:NH2    | 8:XH:123:GLU:OE2   | 2.37                     | 0.58              |
| 25:YA:2056:G:N2    | 51:Y5:4:HIS:O      | 2.36                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:RP:57:THR:CG2   | 35:RP:60:MET:CB    | 2.79                     | 0.57              |
| 8:QH:10:LEU:HD22   | 8:QH:83:ILE:HD11   | 1.86                     | 0.57              |
| 41:RV:29:PRO:HA    | 41:RV:61:VAL:HG13  | 1.86                     | 0.57              |
| 29:RF:122:LYS:O    | 29:RF:124:LEU:N    | 2.37                     | 0.57              |
| 25:YA:2365:G:N7    | 54:Y8:39:LYS:NZ    | 2.51                     | 0.57              |
| 35:RP:94:GLU:HG3   | 35:RP:124:LYS:HB3  | 1.86                     | 0.57              |
| 27:RD:8:PRO:HB3    | 27:RD:14:ARG:HB2   | 1.85                     | 0.57              |
| 25:YA:910:A:H62    | 36:YQ:12:GLN:HA    | 1.69                     | 0.57              |
| 1:XA:666:G:H5'     | 1:XA:726:C:H1'     | 1.85                     | 0.57              |
| 19:QS:36:ARG:O     | 19:QS:38:SER:N     | 2.36                     | 0.57              |
| 25:RA:927:G:H5'    | 25:RA:928:G:OP2    | 2.04                     | 0.57              |
| 30:RG:6:ALA:N      | 50:R4:23:GLU:OE2   | 2.31                     | 0.57              |
| 1:QA:1313:U:P      | 19:QS:6:LYS:HD3    | 2.44                     | 0.57              |
| 35:RP:106:LEU:HD11 | 35:RP:112:LEU:HG   | 1.85                     | 0.57              |
| 3:XC:2:GLY:O       | 3:XC:3:ASN:HB2     | 2.05                     | 0.57              |
| 28:RE:61:ARG:O     | 28:RE:63:LEU:HG    | 2.04                     | 0.57              |
| 25:YA:2467:C:H4'   | 36:YQ:123:HIS:ND1  | 2.19                     | 0.57              |
| 1:XA:1300:G:O2'    | 1:XA:1301:U:O5'    | 2.21                     | 0.57              |
| 24:XY:37:ILE:HD11  | 24:XY:66:ILE:HD11  | 1.85                     | 0.57              |
| 3:XC:26:LYS:HD3    | 10:XJ:45:ARG:HH22  | 1.69                     | 0.57              |
| 1:XA:448:A:OP2     | 1:XA:485:G:N2      | 2.36                     | 0.57              |
| 25:RA:2327:A:H2'   | 25:RA:2328:A:C8    | 2.40                     | 0.57              |
| 45:RZ:91:LEU:H     | 45:RZ:91:LEU:HD23  | 1.69                     | 0.57              |
| 47:R1:50:ARG:NH1   | 47:R1:57:GLU:OE1   | 2.38                     | 0.57              |
| 17:XQ:60:ILE:HB    | 17:XQ:74:LEU:HD23  | 1.86                     | 0.57              |
| 29:YF:178:PRO:HB2  | 29:YF:201:VAL:HG11 | 1.86                     | 0.57              |
| 25:RA:1427:A:H4'   | 25:RA:1428:C:O5'   | 2.04                     | 0.57              |
| 25:YA:994:C:OP1    | 40:YU:53:ARG:NH2   | 2.38                     | 0.57              |
| 32:YI:140:LEU:O    | 32:YI:141:LYS:HD2  | 2.03                     | 0.57              |
| 25:RA:1548:C:N4    | 25:RA:1549:C:N4    | 2.52                     | 0.57              |
| 1:QA:1346:A:OP1    | 9:QI:120:ARG:NH1   | 2.34                     | 0.57              |
| 19:XS:5:LEU:HA     | 19:XS:6:LYS:HE3    | 1.85                     | 0.57              |
| 27:RD:85:ASP:HB2   | 27:RD:92:ILE:HD13  | 1.87                     | 0.57              |
| 24:QY:12:LEU:HB3   | 24:QY:18:VAL:HB    | 1.85                     | 0.57              |
| 1:QA:971:G:N2      | 1:QA:1233:G:H1'    | 2.19                     | 0.57              |
| 45:RZ:19:ARG:NH1   | 45:RZ:84:GLU:O     | 2.37                     | 0.57              |
| 27:YD:79:VAL:HG21  | 27:YD:111:LEU:HD11 | 1.87                     | 0.57              |
| 28:RE:128:SER:OG   | 28:RE:129:HIS:N    | 2.37                     | 0.57              |
| 1:QA:1298:C:H4'    | 1:QA:1299:A:C8     | 2.39                     | 0.57              |
| 1:XA:1483:A:H1'    | 25:YA:1948:G:H1'   | 1.87                     | 0.57              |
| 1:QA:354:G:C6      | 1:QA:355:C:C4      | 2.93                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:956:G:H5''  | 36:YQ:77:LYS:HD2  | 1.87                     | 0.57              |
| 25:YA:2315:G:OP1  | 30:YG:36:LYS:NZ   | 2.37                     | 0.57              |
| 1:QA:501:C:H1'    | 1:QA:549:C:H1'    | 1.86                     | 0.57              |
| 1:QA:1510:U:H2'   | 1:QA:1511:G:C8    | 2.40                     | 0.57              |
| 29:RF:143:ALA:HB1 | 29:RF:148:LEU:HB2 | 1.86                     | 0.57              |
| 1:QA:973:G:H3'    | 1:QA:974:A:H5''   | 1.85                     | 0.57              |
| 25:YA:1252:G:N3   | 40:YU:33:ARG:HD2  | 2.19                     | 0.57              |
| 39:YT:115:ARG:HD3 | 39:YT:115:ARG:H   | 1.70                     | 0.57              |
| 35:YP:105:LEU:O   | 35:YP:107:LYS:N   | 2.36                     | 0.57              |
| 1:QA:1497:G:C2'   | 1:QA:1498:U:H5'   | 2.34                     | 0.57              |
| 1:XA:1157:A:H62   | 1:XA:1178:G:N2    | 2.03                     | 0.57              |
| 22:XW:76:A:O2'    | 25:YA:2394:C:N3   | 2.32                     | 0.57              |
| 1:QA:1492:A:N3    | 25:RA:1913:A:H2   | 2.01                     | 0.57              |
| 19:XS:36:ARG:O    | 19:XS:38:SER:N    | 2.37                     | 0.57              |
| 1:XA:1002:G:N2    | 1:XA:1039:C:O2    | 2.36                     | 0.57              |
| 25:YA:1247:A:OP2  | 35:YP:15:ARG:NH1  | 2.34                     | 0.57              |
| 25:RA:709:U:H2'   | 25:RA:710:G:H8    | 1.70                     | 0.57              |
| 25:RA:1882:C:H5'  | 25:RA:1883:G:OP2  | 2.05                     | 0.57              |
| 1:QA:520:A:N1     | 1:QA:536:C:H1'    | 2.19                     | 0.57              |
| 29:YF:153:SER:HB2 | 29:YF:190:GLU:H   | 1.70                     | 0.57              |
| 31:RH:117:PRO:HB3 | 31:RH:123:PHE:CE1 | 2.40                     | 0.57              |
| 25:RA:2310:A:N6   | 30:RG:79:ASN:OD1  | 2.37                     | 0.57              |
| 9:XI:15:ALA:HB2   | 9:XI:65:VAL:HG23  | 1.86                     | 0.57              |
| 1:XA:975:A:O2'    | 14:YN:32:SER:HB3  | 2.04                     | 0.57              |
| 36:YQ:89:ASN:O    | 36:YQ:92:GLY:N    | 2.35                     | 0.57              |
| 4:XD:108:LEU:HD21 | 4:XD:183:GLY:HA3  | 1.86                     | 0.57              |
| 30:YG:96:ARG:O    | 30:YG:98:ARG:N    | 2.37                     | 0.57              |
| 13:QM:53:VAL:HG12 | 13:QM:57:ARG:HD3  | 1.87                     | 0.57              |
| 25:RA:521:G:H2'   | 25:RA:522:G:H8    | 1.70                     | 0.57              |
| 4:QD:125:HIS:ND1  | 4:QD:152:SER:OG   | 2.29                     | 0.57              |
| 1:QA:737:A:H5''   | 6:QF:92:LYS:HG3   | 1.87                     | 0.57              |
| 46:R0:36:ILE:HA   | 46:R0:60:PHE:HA   | 1.87                     | 0.57              |
| 1:QA:1347:G:N2    | 1:QA:1373:G:H2'   | 2.20                     | 0.57              |
| 35:RP:52:GLU:HB2  | 35:RP:55:ARG:HB3  | 1.86                     | 0.57              |
| 31:YH:126:PRO:HB2 | 31:YH:127:GLU:HA  | 1.86                     | 0.57              |
| 25:RA:521:G:H2'   | 25:RA:522:G:C8    | 2.39                     | 0.57              |
| 1:QA:1228:C:H4'   | 13:QM:116:THR:HA  | 1.87                     | 0.57              |
| 42:YW:35:ILE:HG23 | 51:Y5:28:PRO:HD2  | 1.87                     | 0.57              |
| 25:YA:1405:U:H2'  | 25:YA:1406:U:C6   | 2.39                     | 0.57              |
| 25:YA:2357:U:OP1  | 46:Y0:20:ARG:NH1  | 2.36                     | 0.57              |
| 39:YT:26:ASP:HB3  | 39:YT:92:GLY:H    | 1.69                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:XA:833:U:H2'    | 1:XA:834:C:C6      | 2.40                     | 0.57              |
| 25:YA:1270:C:H5'' | 25:YA:1271:G:H5'   | 1.87                     | 0.57              |
| 8:XH:10:LEU:HD22  | 8:XH:83:ILE:HD11   | 1.86                     | 0.57              |
| 28:RE:37:ARG:HG3  | 28:RE:46:ALA:HB3   | 1.85                     | 0.56              |
| 25:YA:74:A:H4'    | 25:YA:75:G:O5'     | 2.05                     | 0.56              |
| 47:R1:87:PRO:HA   | 47:R1:90:ILE:HG22  | 1.87                     | 0.56              |
| 39:RT:125:ARG:NH1 | 39:RT:128:GLU:OE1  | 2.38                     | 0.56              |
| 38:RS:49:VAL:HG22 | 38:RS:80:LEU:HD12  | 1.87                     | 0.56              |
| 39:RT:74:ARG:HD3  | 39:RT:76:PHE:CZ    | 2.40                     | 0.56              |
| 6:XF:101:ALA:HA   | 18:XR:28:GLU:HB3   | 1.84                     | 0.56              |
| 8:XH:103:VAL:HG21 | 8:XH:110:ALA:HB2   | 1.87                     | 0.56              |
| 3:XC:131:ARG:NH2  | 3:XC:167:TRP:O     | 2.38                     | 0.56              |
| 14:YN:12:ARG:HG2  | 14:YN:14:PRO:HD3   | 1.86                     | 0.56              |
| 14:YN:41:ARG:CZ   | 14:YN:42:ILE:HD11  | 2.36                     | 0.56              |
| 25:RA:1223:G:H5'  | 25:RA:1224:C:OP2   | 2.05                     | 0.56              |
| 1:XA:1391:U:H2'   | 1:XA:1392:G:C8     | 2.39                     | 0.56              |
| 41:YV:4:ILE:HG22  | 41:YV:39:LEU:HD13  | 1.86                     | 0.56              |
| 25:YA:2010:G:H5'' | 42:YW:42:ARG:HB2   | 1.87                     | 0.56              |
| 1:XA:531:U:O4     | 24:XY:29:ARG:NH2   | 2.28                     | 0.56              |
| 19:QS:64:GLU:O    | 19:QS:66:MET:N     | 2.37                     | 0.56              |
| 25:RA:247:G:OP2   | 25:RA:249:C:N4     | 2.37                     | 0.56              |
| 28:YE:74:PRO:HG2  | 28:YE:78:LEU:HD23  | 1.87                     | 0.56              |
| 25:RA:1907:G:O2'  | 25:RA:1908:C:H5'   | 2.05                     | 0.56              |
| 25:RA:2271:G:OP1  | 46:R0:18:ALA:HB1   | 2.05                     | 0.56              |
| 1:XA:1075:C:OP1   | 2:XB:179:LYS:HE2   | 2.05                     | 0.56              |
| 25:YA:530:G:N1    | 25:YA:2023:G:OP1   | 2.25                     | 0.56              |
| 10:XJ:48:THR:HA   | 10:XJ:62:HIS:HB3   | 1.87                     | 0.56              |
| 45:RZ:157:LEU:CB  | 45:RZ:161:VAL:HG11 | 2.33                     | 0.56              |
| 9:XI:32:ASP:HB2   | 9:XI:35:GLU:HB2    | 1.87                     | 0.56              |
| 11:XK:54:ARG:HH11 | 11:XK:54:ARG:HG2   | 1.70                     | 0.56              |
| 25:RA:848:G:H2'   | 25:RA:849:A:C8     | 2.40                     | 0.56              |
| 1:QA:1379:G:N2    | 1:QA:1381:U:O4     | 2.37                     | 0.56              |
| 1:QA:1131:G:H1    | 1:QA:1143:G:H21    | 1.52                     | 0.56              |
| 2:XB:119:GLU:OE2  | 2:XB:153:ARG:NH2   | 2.38                     | 0.56              |
| 46:Y0:4:LYS:H     | 46:Y0:5:LYS:HB3    | 1.69                     | 0.56              |
| 1:XA:972:C:O3'    | 10:XJ:57:LYS:HG2   | 2.06                     | 0.56              |
| 25:RA:1265:A:OP1  | 25:RA:1265:A:H8    | 1.88                     | 0.56              |
| 1:QA:382:A:H2'    | 1:QA:383:A:H8      | 1.70                     | 0.56              |
| 25:YA:574:C:O2    | 28:YE:145:LYS:NZ   | 2.36                     | 0.56              |
| 25:RA:576:U:H2'   | 25:RA:577:G:C8     | 2.41                     | 0.56              |
| 4:QD:195:ALA:O    | 6:XF:16:GLN:HB3    | 2.05                     | 0.56              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:RA:1027:A:C2     | 25:RA:2488:A:H5'   | 2.39                     | 0.56              |
| 43:RX:8:ILE:O       | 48:R2:36:ARG:NH2   | 2.38                     | 0.56              |
| 25:RA:974(A):C:H4'  | 25:RA:974(A):C:OP2 | 2.05                     | 0.56              |
| 2:XB:189:ASP:O      | 2:XB:191:ASP:N     | 2.38                     | 0.56              |
| 5:XE:19:MET:HA      | 5:XE:24:ARG:HA     | 1.86                     | 0.56              |
| 1:QA:1493:A:H8      | 1:QA:1493:A:O5'    | 1.88                     | 0.56              |
| 31:YH:7:LEU:HD22    | 31:YH:69:ARG:HG2   | 1.88                     | 0.56              |
| 25:YA:2232:U:OP2    | 47:Y1:40:ARG:NH2   | 2.37                     | 0.56              |
| 25:RA:1142(A):A:H4' | 33:RN:25:ARG:HH22  | 1.68                     | 0.56              |
| 25:RA:1270:C:H5''   | 25:RA:1271:G:H5'   | 1.87                     | 0.56              |
| 40:YU:93:LYS:HD3    | 40:YU:93:LYS:N     | 2.21                     | 0.56              |
| 36:YQ:54:MET:HE1    | 36:YQ:118:LEU:HD23 | 1.85                     | 0.56              |
| 1:QA:67:C:H2'       | 1:QA:68:G:C8       | 2.41                     | 0.56              |
| 25:RA:987:G:O2'     | 25:RA:1000:A:N3    | 2.37                     | 0.56              |
| 17:QQ:90:ILE:O      | 17:QQ:94:ASN:ND2   | 2.39                     | 0.56              |
| 10:QJ:38:ILE:HB     | 10:QJ:71:LEU:HB3   | 1.86                     | 0.56              |
| 32:YI:98:ALA:HA     | 32:YI:109:ILE:HD11 | 1.87                     | 0.56              |
| 22:XW:54:U:H3       | 22:XW:58:A:N6      | 2.04                     | 0.56              |
| 10:XJ:34:VAL:HG22   | 10:XJ:74:ILE:HG22  | 1.87                     | 0.56              |
| 25:RA:2346:A:H2     | 52:R6:25:LYS:HB3   | 1.70                     | 0.56              |
| 12:QL:126:LYS:H     | 12:QL:126:LYS:HD3  | 1.70                     | 0.56              |
| 25:RA:2356:C:H4'    | 46:R0:20:ARG:HG3   | 1.87                     | 0.56              |
| 5:XE:8:GLU:HG2      | 5:XE:34:VAL:HG22   | 1.87                     | 0.56              |
| 3:XC:82:GLU:HG3     | 3:XC:83:ARG:H      | 1.70                     | 0.56              |
| 27:RD:146:GLU:HB2   | 27:RD:189:CYS:HB3  | 1.87                     | 0.56              |
| 25:RA:1094:U:O2'    | 25:RA:1096:A:OP1   | 2.24                     | 0.56              |
| 25:YA:1096:A:C5     | 25:YA:1097:U:H1'   | 2.41                     | 0.56              |
| 45:RZ:59:LEU:HD12   | 45:RZ:60:GLU:CA    | 2.36                     | 0.56              |
| 35:RP:9:ASN:O       | 35:RP:11:GLY:N     | 2.39                     | 0.56              |
| 1:QA:1224:G:O2'     | 1:QA:1322:C:OP1    | 2.23                     | 0.56              |
| 25:YA:1761:C:C4     | 25:YA:1762:A:N1    | 2.73                     | 0.56              |
| 25:RA:1657:C:H2'    | 25:RA:1658:C:C6    | 2.39                     | 0.56              |
| 25:RA:2091:U:C5'    | 25:RA:2092:U:H5''  | 2.36                     | 0.56              |
| 1:QA:436:C:H2'      | 1:QA:437:U:C6      | 2.41                     | 0.56              |
| 24:QY:89:GLU:HG3    | 24:QY:90:ASP:O     | 2.06                     | 0.56              |
| 52:R6:34:LEU:HD11   | 52:R6:50:ARG:HH21  | 1.71                     | 0.56              |
| 25:YA:911:A:H2'     | 36:YQ:9:TYR:OH     | 2.06                     | 0.56              |
| 11:QK:84:VAL:HG23   | 11:QK:110:ASP:HA   | 1.88                     | 0.56              |
| 31:RH:24:VAL:HG22   | 31:RH:35:VAL:HB    | 1.88                     | 0.56              |
| 1:QA:279:A:H5''     | 1:QA:281:G:O4'     | 2.06                     | 0.56              |
| 6:XF:55:ASP:HB2     | 6:XF:86:ARG:HH12   | 1.69                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:RE:37:ARG:HD3   | 28:RE:44:TYR:OH    | 2.06                     | 0.56              |
| 25:RA:2712:U:OP1   | 25:RA:2714:G:H4'   | 2.05                     | 0.56              |
| 35:YP:52:GLU:HG2   | 35:YP:55:ARG:NE    | 2.16                     | 0.56              |
| 25:YA:6:A:N1       | 25:YA:7:G:C5       | 2.74                     | 0.56              |
| 45:RZ:116:VAL:O    | 45:RZ:118:GLN:NE2  | 2.39                     | 0.56              |
| 25:RA:1721:G:H8    | 25:RA:1741:A:H62   | 1.53                     | 0.56              |
| 1:QA:1316:G:H5''   | 14:QN:17:LYS:HE3   | 1.87                     | 0.56              |
| 4:XD:199:ASN:O     | 4:XD:201:GLN:N     | 2.35                     | 0.56              |
| 1:QA:985:C:H2'     | 1:QA:986:A:H8      | 1.70                     | 0.56              |
| 45:RZ:124:ILE:HD11 | 45:RZ:165:VAL:HG11 | 1.87                     | 0.56              |
| 25:RA:2291:U:H2'   | 25:RA:2292:C:C6    | 2.41                     | 0.56              |
| 25:RA:1056:G:H4'   | 25:RA:1086:A:H1'   | 1.87                     | 0.56              |
| 29:RF:125:LEU:H    | 29:RF:125:LEU:HD23 | 1.70                     | 0.56              |
| 44:YY:39:VAL:HG23  | 44:YY:41:GLY:H     | 1.70                     | 0.56              |
| 27:YD:35:LYS:HG2   | 27:YD:64:ILE:H     | 1.69                     | 0.56              |
| 1:QA:1236:A:C2     | 1:QA:1237:C:C2     | 2.93                     | 0.56              |
| 28:YE:8:LYS:HB3    | 28:YE:193:GLY:H    | 1.71                     | 0.56              |
| 1:XA:173:U:O2      | 1:XA:197:A:N6      | 2.37                     | 0.56              |
| 1:QA:982:U:H5''    | 14:QN:6:LEU:HD11   | 1.86                     | 0.56              |
| 1:XA:1158:C:N4     | 1:XA:1160:G:C5     | 2.74                     | 0.56              |
| 25:RA:58:G:H1      | 25:RA:69:C:N4      | 2.02                     | 0.56              |
| 25:RA:58:G:N2      | 25:RA:69:C:H5      | 2.00                     | 0.56              |
| 1:QA:1322:C:O2'    | 1:QA:1323:G:OP2    | 2.21                     | 0.56              |
| 31:YH:127:GLU:HG3  | 31:YH:128:PRO:HD2  | 1.87                     | 0.56              |
| 1:QA:382:A:H2'     | 1:QA:383:A:C8      | 2.41                     | 0.56              |
| 25:RA:854:G:H5'    | 25:RA:855:G:OP2    | 2.06                     | 0.56              |
| 2:XB:80:ILE:HD11   | 2:XB:211:ILE:HG22  | 1.88                     | 0.56              |
| 19:QS:42:PRO:HG3   | 50:R4:60:GLN:HG3   | 1.87                     | 0.56              |
| 25:YA:2472:G:H5'   | 25:YA:2473:U:H5''  | 1.85                     | 0.56              |
| 31:YH:12:PRO:HG3   | 31:YH:48:GLY:HA2   | 1.88                     | 0.56              |
| 13:QM:23:TYR:CD1   | 13:QM:71:ARG:HD2   | 2.40                     | 0.56              |
| 27:YD:159:ALA:H    | 27:YD:196:VAL:HG11 | 1.71                     | 0.56              |
| 28:RE:47:VAL:O     | 28:RE:49:LEU:HD13  | 2.06                     | 0.56              |
| 1:QA:1492:A:O5'    | 1:QA:1492:A:H8     | 1.89                     | 0.56              |
| 30:RG:68:PRO:HA    | 30:RG:92:VAL:HB    | 1.88                     | 0.56              |
| 10:QJ:50:ILE:HD13  | 10:QJ:60:ARG:HD3   | 1.88                     | 0.56              |
| 31:YH:6:ARG:HB3    | 31:YH:54:ARG:HH12  | 1.71                     | 0.56              |
| 10:QJ:4:ILE:HA     | 10:QJ:100:THR:HG22 | 1.87                     | 0.56              |
| 18:QR:22:VAL:HG22  | 18:QR:23:LYS:H     | 1.70                     | 0.56              |
| 31:RH:30:LYS:HB3   | 31:RH:136:ILE:HG21 | 1.86                     | 0.56              |
| 10:XJ:10:GLY:HA3   | 10:XJ:16:LEU:HD21  | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:YW:29:LEU:HD21 | 42:YW:33:ARG:HH21 | 1.70                     | 0.56              |
| 25:RA:990:A:C6    | 25:RA:1186:G:H1'  | 2.40                     | 0.56              |
| 22:QW:15:G:H2'    | 22:QW:59:A:C2     | 2.40                     | 0.56              |
| 26:YB:56:G:H5'    | 30:YG:27:ASN:ND2  | 2.21                     | 0.56              |
| 25:YA:2406:U:N3   | 35:YP:73:GLY:O    | 2.37                     | 0.55              |
| 1:QA:750:G:N3     | 15:QO:23:GLY:HA3  | 2.22                     | 0.55              |
| 26:RB:64:C:H2'    | 26:RB:65:C:C6     | 2.42                     | 0.55              |
| 4:QD:73:ARG:O     | 4:QD:77:ASN:ND2   | 2.40                     | 0.55              |
| 1:QA:250:A:H4'    | 1:QA:251:G:O5'    | 2.05                     | 0.55              |
| 45:YZ:151:HIS:O   | 45:YZ:154:ASP:HB3 | 2.05                     | 0.55              |
| 1:XA:612:C:O2     | 1:XA:629:G:N2     | 2.39                     | 0.55              |
| 5:XE:13:ILE:H     | 5:XE:13:ILE:HD13  | 1.70                     | 0.55              |
| 18:XR:31:LEU:HD13 | 18:XR:65:ILE:HD13 | 1.88                     | 0.55              |
| 25:YA:975:G:N2    | 25:YA:990:A:O4'   | 2.38                     | 0.55              |
| 25:RA:2420:C:OP2  | 54:R8:33:ASN:HA   | 2.05                     | 0.55              |
| 25:YA:1025:G:OP1  | 25:YA:1025:G:H8   | 1.88                     | 0.55              |
| 36:RQ:80:GLU:HG2  | 36:RQ:81:VAL:H    | 1.72                     | 0.55              |
| 25:RA:958:U:OP2   | 36:RQ:14:ARG:NH1  | 2.39                     | 0.55              |
| 17:XQ:12:SER:HB3  | 17:XQ:20:THR:HB   | 1.89                     | 0.55              |
| 1:QA:1435:G:H2'   | 1:QA:1436:U:C6    | 2.41                     | 0.55              |
| 1:QA:1008:C:H42   | 1:QA:1021:G:H1    | 1.55                     | 0.55              |
| 1:QA:349:A:C3'    | 1:QA:350:G:H5''   | 2.35                     | 0.55              |
| 2:XB:9:GLU:HG2    | 2:XB:48:MET:HG3   | 1.88                     | 0.55              |
| 25:YA:1230:C:H2'  | 25:YA:1231:G:C8   | 2.40                     | 0.55              |
| 1:QA:501:C:H2'    | 1:QA:502:G:H8     | 1.71                     | 0.55              |
| 25:RA:2680:C:H5'  | 28:RE:189:PRO:HA  | 1.87                     | 0.55              |
| 38:YS:19:LYS:O    | 38:YS:21:THR:N    | 2.35                     | 0.55              |
| 27:RD:101:GLU:OE1 | 27:RD:103:ARG:NH1 | 2.39                     | 0.55              |
| 38:YS:93:LYS:HG2  | 38:YS:95:HIS:HB2  | 1.88                     | 0.55              |
| 1:XA:267:C:OP1    | 17:XQ:67:LYS:HB2  | 2.07                     | 0.55              |
| 31:RH:45:VAL:HG13 | 31:RH:46:GLU:H    | 1.71                     | 0.55              |
| 9:QI:2:GLU:H      | 9:QI:20:ARG:HH11  | 1.51                     | 0.55              |
| 31:RH:86:GLU:HG3  | 31:RH:165:ALA:HB2 | 1.88                     | 0.55              |
| 44:RY:96:ILE:HG12 | 44:RY:101:LYS:HG3 | 1.87                     | 0.55              |
| 1:QA:960:U:O2'    | 1:QA:1223:C:H4'   | 2.06                     | 0.55              |
| 3:QC:52:LEU:H     | 3:QC:52:LEU:HD23  | 1.72                     | 0.55              |
| 28:YE:37:ARG:HA   | 28:YE:42:ASP:OD2  | 2.06                     | 0.55              |
| 42:RW:59:VAL:HA   | 42:RW:64:MET:H    | 1.72                     | 0.55              |
| 27:RD:44:ASN:OD1  | 27:RD:44:ASN:N    | 2.39                     | 0.55              |
| 30:YG:27:ASN:HB3  | 30:YG:30:GLU:HG3  | 1.88                     | 0.55              |
| 25:RA:1416:G:N2   | 25:RA:1582:C:O2   | 2.36                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:XO:26:GLU:OE2   | 15:XO:77:ARG:NH1   | 2.39                     | 0.55              |
| 30:YG:131:TYR:HB3  | 30:YG:159:VAL:HG13 | 1.88                     | 0.55              |
| 25:RA:629:G:N3     | 25:RA:639:U:O2'    | 2.38                     | 0.55              |
| 1:QA:17:U:H2'      | 1:QA:18:C:C6       | 2.42                     | 0.55              |
| 1:QA:765:G:N2      | 1:QA:813:U:OP2     | 2.38                     | 0.55              |
| 51:Y5:41:PRO:O     | 51:Y5:44:THR:OG1   | 2.23                     | 0.55              |
| 36:YQ:31:ASP:H     | 36:YQ:107:ALA:HB2  | 1.70                     | 0.55              |
| 31:RH:9:ILE:O      | 31:RH:69:ARG:NE    | 2.39                     | 0.55              |
| 45:RZ:121:HIS:H    | 45:RZ:171:ILE:HG12 | 1.72                     | 0.55              |
| 29:YF:102:PRO:HB2  | 29:YF:105:VAL:HG23 | 1.89                     | 0.55              |
| 9:QI:28:VAL:HG21   | 9:QI:63:ILE:N      | 2.22                     | 0.55              |
| 1:QA:718:G:N2      | 18:QR:82:THR:HG23  | 2.22                     | 0.55              |
| 1:XA:1122:U:O4     | 1:XA:1123:A:N6     | 2.40                     | 0.55              |
| 26:YB:44:G:H1'     | 26:YB:47:C:N4      | 2.21                     | 0.55              |
| 1:QA:404:U:H2'     | 1:QA:405:U:H6      | 1.72                     | 0.55              |
| 45:RZ:69:THR:HG22  | 45:RZ:90:VAL:HA    | 1.89                     | 0.55              |
| 25:YA:1693:U:O2'   | 27:YD:14:ARG:NH2   | 2.40                     | 0.55              |
| 15:QO:87:ILE:HG22  | 15:QO:88:ARG:H     | 1.72                     | 0.55              |
| 27:YD:26:LYS:H     | 27:YD:26:LYS:HD2   | 1.71                     | 0.55              |
| 12:XL:126:LYS:H    | 12:XL:126:LYS:HD3  | 1.72                     | 0.55              |
| 25:RA:1190:G:H5'   | 35:RP:32:THR:HA    | 1.87                     | 0.55              |
| 25:YA:2128:C:N4    | 25:YA:2159:G:O6    | 2.40                     | 0.55              |
| 25:YA:532:A:N1     | 25:YA:2035:G:N2    | 2.54                     | 0.55              |
| 32:YI:128:LEU:HD22 | 32:YI:140:LEU:HD22 | 1.89                     | 0.55              |
| 32:RI:125:GLU:CA   | 32:RI:141:LYS:HB3  | 2.24                     | 0.55              |
| 1:QA:1348:U:H3     | 1:QA:1374:A:H2     | 1.52                     | 0.55              |
| 9:QI:27:THR:HG21   | 9:QI:32:ASP:HA     | 1.88                     | 0.55              |
| 25:RA:2144:U:O2'   | 25:RA:2145:C:O5'   | 2.23                     | 0.55              |
| 25:RA:2790:A:H2'   | 25:RA:2791:C:H5'   | 1.89                     | 0.55              |
| 15:QO:3:ILE:H      | 15:QO:3:ILE:HD13   | 1.72                     | 0.55              |
| 3:XC:134:ILE:HG23  | 3:XC:151:VAL:HB    | 1.89                     | 0.55              |
| 32:YI:76:THR:OG1   | 32:YI:77:LEU:N     | 2.39                     | 0.55              |
| 23:QX:13:A:C3'     | 23:QX:14:A:H5''    | 2.36                     | 0.55              |
| 2:QB:187:LEU:HA    | 2:QB:201:ILE:HB    | 1.87                     | 0.55              |
| 39:RT:3:ARG:HG2    | 39:RT:6:LEU:HB2    | 1.88                     | 0.55              |
| 2:QB:219:VAL:HA    | 2:QB:222:ILE:HD12  | 1.89                     | 0.55              |
| 47:R1:80:LEU:HD13  | 47:R1:80:LEU:H     | 1.72                     | 0.55              |
| 9:QI:15:ALA:HB2    | 9:QI:65:VAL:HG23   | 1.88                     | 0.55              |
| 31:YH:64:LEU:O     | 31:YH:68:THR:OG1   | 2.23                     | 0.55              |
| 1:QA:1348:U:N3     | 1:QA:1374:A:H2     | 2.05                     | 0.55              |
| 40:YU:92:ARG:HH12  | 41:YV:11:GLN:H     | 1.53                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:QA:1060:C:H5''   | 10:QJ:51:ARG:HG2   | 1.88                     | 0.55              |
| 25:YA:1762:A:C4'   | 25:YA:1763:G:OP2   | 2.54                     | 0.55              |
| 32:YI:86:THR:HG22  | 32:YI:122:GLU:HG3  | 1.89                     | 0.55              |
| 20:XT:29:LYS:O     | 20:XT:33:ILE:HG12  | 2.06                     | 0.55              |
| 32:YI:3:VAL:HG12   | 32:YI:38:LEU:HA    | 1.88                     | 0.55              |
| 25:RA:1375:C:H2'   | 25:RA:1376:C:H6    | 1.71                     | 0.55              |
| 25:RA:1403:C:H5''  | 25:RA:1471:A:H1'   | 1.89                     | 0.55              |
| 48:Y2:18:PRO:HA    | 48:Y2:21:LEU:HB2   | 1.88                     | 0.55              |
| 2:QB:76:GLN:HG3    | 2:QB:208:ILE:HG12  | 1.89                     | 0.55              |
| 28:RE:80:GLU:O     | 28:RE:82:ARG:N     | 2.39                     | 0.55              |
| 28:YE:60:ASN:CB    | 28:YE:62:PRO:HD2   | 2.37                     | 0.55              |
| 47:R1:53:VAL:HG22  | 47:R1:74:VAL:HG13  | 1.88                     | 0.55              |
| 31:RH:3:ARG:HH11   | 31:RH:6:ARG:HE     | 1.54                     | 0.55              |
| 25:YA:1755:A:N6    | 25:YA:2694:G:O2'   | 2.40                     | 0.55              |
| 25:RA:465:G:H2'    | 25:RA:466:A:C8     | 2.42                     | 0.55              |
| 20:XT:26:ASN:HB2   | 20:XT:71:THR:HG23  | 1.87                     | 0.55              |
| 2:XB:7:VAL:HG13    | 2:XB:8:LYS:H       | 1.72                     | 0.55              |
| 3:XC:92:ALA:HA     | 3:XC:95:THR:HB     | 1.88                     | 0.55              |
| 1:XA:534:U:H5'     | 1:XA:535:A:OP2     | 2.06                     | 0.55              |
| 25:RA:264:C:HO2'   | 25:RA:265:A:H2'    | 1.70                     | 0.55              |
| 25:RA:517:C:OP1    | 51:R5:16:ARG:NH2   | 2.39                     | 0.55              |
| 12:XL:23:LYS:H     | 12:XL:23:LYS:HD3   | 1.72                     | 0.55              |
| 22:QV:1:C:HO5'     | 22:QV:1:C:H6       | 1.54                     | 0.55              |
| 25:RA:2031:A:O2'   | 25:RA:2454:G:N2    | 2.34                     | 0.55              |
| 31:RH:11:VAL:HG23  | 31:RH:13:LYS:HG2   | 1.89                     | 0.55              |
| 25:RA:661:C:H1'    | 35:RP:12:ALA:HA    | 1.88                     | 0.55              |
| 42:RW:18:ARG:NH1   | 42:RW:76:VAL:O     | 2.40                     | 0.55              |
| 25:YA:1400:G:H2'   | 25:YA:1401:G:H8    | 1.71                     | 0.55              |
| 25:RA:1693:U:O2'   | 27:RD:14:ARG:NH2   | 2.40                     | 0.55              |
| 1:QA:1497:G:H2'    | 1:QA:1498:U:H5'    | 1.88                     | 0.55              |
| 27:YD:106:ILE:HD11 | 27:YD:196:VAL:HG13 | 1.89                     | 0.55              |
| 6:XF:11:ASN:HB3    | 6:XF:14:LEU:HG     | 1.89                     | 0.55              |
| 30:RG:125:PHE:HB3  | 30:RG:166:ASP:HB2  | 1.89                     | 0.55              |
| 1:XA:1137:C:H4'    | 1:XA:1138:G:O5'    | 2.07                     | 0.55              |
| 25:RA:878:A:N6     | 25:RA:899:A:O2'    | 2.40                     | 0.55              |
| 25:RA:455:C:N3     | 25:RA:473:G:H5'    | 2.21                     | 0.55              |
| 11:XK:98:LEU:O     | 11:XK:101:SER:OG   | 2.21                     | 0.55              |
| 25:RA:807:U:OP2    | 35:RP:41:ARG:NH1   | 2.40                     | 0.55              |
| 44:RY:43:ASN:HB3   | 44:RY:64:GLU:HA    | 1.89                     | 0.55              |
| 30:YG:16:ARG:HE    | 30:YG:31:VAL:HG11  | 1.72                     | 0.55              |
| 2:QB:102:LEU:HD23  | 2:QB:182:ILE:HD12  | 1.88                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:QH:69:ARG:NH1   | 8:QH:75:ARG:O      | 2.40                     | 0.55              |
| 1:XA:736:C:OP1    | 18:XR:68:LYS:NZ    | 2.33                     | 0.55              |
| 16:XP:71:ARG:HG3  | 16:XP:80:PHE:HE1   | 1.72                     | 0.55              |
| 32:YI:2:LYS:HA    | 32:YI:20:ASP:HA    | 1.89                     | 0.55              |
| 45:RZ:58:VAL:CG1  | 45:RZ:60:GLU:HG2   | 2.36                     | 0.54              |
| 25:RA:2689:U:H5'' | 25:RA:2713:A:C2    | 2.42                     | 0.54              |
| 25:RA:1688:U:O2   | 25:RA:1700:A:H5'   | 2.06                     | 0.54              |
| 25:RA:907:U:HO2'  | 36:RQ:101:ARG:HH22 | 1.51                     | 0.54              |
| 25:RA:2816:C:O2   | 25:RA:2883:A:O2'   | 2.23                     | 0.54              |
| 25:YA:2144:U:O2'  | 25:YA:2145:C:O5'   | 2.22                     | 0.54              |
| 47:Y1:8:SER:HB3   | 47:Y1:66:HIS:CD2   | 2.42                     | 0.54              |
| 25:YA:883:G:H1    | 25:YA:893:C:H42    | 1.53                     | 0.54              |
| 25:RA:6:A:H2'     | 25:RA:7:G:H8       | 1.71                     | 0.54              |
| 31:RH:89:ILE:HD12 | 31:RH:129:THR:HA   | 1.90                     | 0.54              |
| 35:YP:59:LEU:HD21 | 54:Y8:10:ALA:HA    | 1.89                     | 0.54              |
| 7:XG:2:ALA:O      | 7:XG:3:ARG:HB2     | 2.07                     | 0.54              |
| 1:QA:1392:G:H21   | 1:QA:1502:A:H8     | 1.56                     | 0.54              |
| 54:Y8:61:LEU:HD12 | 54:Y8:62:LEU:H     | 1.72                     | 0.54              |
| 25:RA:1754:C:P    | 39:RT:96:ARG:HH12  | 2.30                     | 0.54              |
| 21:XU:8:THR:HG22  | 21:XU:10:ARG:H     | 1.71                     | 0.54              |
| 1:QA:354:G:C2     | 1:QA:355:C:C6      | 2.95                     | 0.54              |
| 1:QA:1152:A:H2'   | 1:QA:1153:C:C6     | 2.41                     | 0.54              |
| 30:RG:41:GLN:NE2  | 30:RG:154:GLY:O    | 2.34                     | 0.54              |
| 31:RH:150:ALA:O   | 31:RH:152:ARG:N    | 2.39                     | 0.54              |
| 6:XF:7:ASN:N      | 6:XF:7:ASN:HD22    | 2.06                     | 0.54              |
| 25:RA:373:U:H2'   | 25:RA:374:A:H8     | 1.72                     | 0.54              |
| 9:QI:121:ARG:NH1  | 9:QI:122:ALA:O     | 2.40                     | 0.54              |
| 19:QS:72:GLY:HA2  | 19:QS:75:ALA:HB3   | 1.88                     | 0.54              |
| 25:YA:2393:A:H4'  | 35:YP:62:LEU:H     | 1.73                     | 0.54              |
| 25:RA:2445:G:H2'  | 25:RA:2446:G:H5'   | 1.89                     | 0.54              |
| 7:QG:86:GLN:NE2   | 22:QW:31:G:N2      | 2.44                     | 0.54              |
| 1:XA:960:U:O2'    | 1:XA:961:U:P       | 2.65                     | 0.54              |
| 50:R4:39:CYS:O    | 50:R4:40:HIS:ND1   | 2.40                     | 0.54              |
| 25:YA:2692:C:H2'  | 25:YA:2693:A:C8    | 2.42                     | 0.54              |
| 10:XJ:4:ILE:HB    | 10:XJ:74:ILE:HD11  | 1.88                     | 0.54              |
| 28:YE:8:LYS:HG2   | 28:YE:192:ASN:HA   | 1.88                     | 0.54              |
| 9:QI:2:GLU:HG3    | 9:QI:3:GLN:H       | 1.72                     | 0.54              |
| 6:XF:22:GLU:O     | 6:XF:26:ILE:HG13   | 2.07                     | 0.54              |
| 25:YA:760:G:H2'   | 25:YA:761:A:O4'    | 2.07                     | 0.54              |
| 41:RV:59:ALA:HB2  | 41:RV:96:ILE:HD13  | 1.89                     | 0.54              |
| 1:XA:1145:C:H4'   | 1:XA:1146:A:H5'    | 1.88                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:QT:10:LEU:HD22  | 20:QT:11:SER:N     | 2.22                     | 0.54              |
| 29:YF:42:ALA:O     | 29:YF:45:ARG:HB2   | 2.07                     | 0.54              |
| 25:YA:1903:G:OP2   | 27:YD:241:PRO:HB2  | 2.07                     | 0.54              |
| 42:RW:12:ILE:HD13  | 42:RW:17:VAL:HG13  | 1.89                     | 0.54              |
| 1:QA:1493:A:H1'    | 24:QY:55:PRO:HD2   | 1.88                     | 0.54              |
| 52:R6:8:LYS:HB2    | 52:R6:27:LYS:HB2   | 1.88                     | 0.54              |
| 25:YA:1112:G:H5'   | 31:YH:3:ARG:HE     | 1.72                     | 0.54              |
| 25:YA:1401:G:H2'   | 25:YA:1402:C:C6    | 2.43                     | 0.54              |
| 1:XA:1255:G:OP1    | 10:XJ:45:ARG:NH2   | 2.41                     | 0.54              |
| 25:YA:518:G:H4'    | 42:YW:18:ARG:NH1   | 2.21                     | 0.54              |
| 27:RD:130:ALA:HA   | 27:RD:192:THR:HA   | 1.89                     | 0.54              |
| 48:Y2:47:ASN:O     | 48:Y2:49:LYS:N     | 2.32                     | 0.54              |
| 25:YA:876:C:H2'    | 25:YA:877:U:O4'    | 2.06                     | 0.54              |
| 25:RA:528:A:HO2'   | 25:RA:2042:A:H2    | 1.56                     | 0.54              |
| 1:QA:701:C:H4'     | 1:QA:701:C:OP1     | 2.08                     | 0.54              |
| 1:XA:652:U:H1'     | 1:XA:653:A:C2      | 2.43                     | 0.54              |
| 1:XA:1191:A:C5'    | 3:XC:4:LYS:HE2     | 2.37                     | 0.54              |
| 25:YA:986:C:C2'    | 25:YA:987:G:C5'    | 2.82                     | 0.54              |
| 35:YP:11:GLY:C     | 35:YP:13:ASN:H     | 2.11                     | 0.54              |
| 45:RZ:118:GLN:O    | 45:RZ:120:ILE:HG22 | 2.07                     | 0.54              |
| 22:QW:16:C:H4'     | 22:QW:60:U:H4'     | 1.88                     | 0.54              |
| 23:QX:10:G:C2'     | 23:QX:11:U:H5''    | 2.38                     | 0.54              |
| 5:XE:101:ILE:HG13  | 5:XE:119:LEU:HD23  | 1.88                     | 0.54              |
| 1:QA:735:C:H2'     | 1:QA:736:C:H6      | 1.72                     | 0.54              |
| 44:YY:88:LYS:O     | 44:YY:90:LEU:N     | 2.39                     | 0.54              |
| 2:QB:80:ILE:HD13   | 2:QB:212:GLN:HA    | 1.89                     | 0.54              |
| 32:RI:131:LYS:HB3  | 32:RI:132:PRO:HA   | 1.88                     | 0.54              |
| 13:XM:44:ARG:HB3   | 13:XM:46:LYS:HB3   | 1.88                     | 0.54              |
| 5:XE:33:VAL:HG12   | 5:XE:112:LEU:HD12  | 1.90                     | 0.54              |
| 33:RN:39:ARG:HH21  | 33:RN:41:ASP:HB2   | 1.73                     | 0.54              |
| 43:YX:36:LYS:HD3   | 43:YX:56:THR:HG23  | 1.90                     | 0.54              |
| 3:QC:11:ARG:O      | 3:QC:13:GLY:N      | 2.39                     | 0.54              |
| 45:YZ:120:ILE:HG23 | 45:YZ:171:ILE:HA   | 1.88                     | 0.54              |
| 25:RA:2787:C:O2'   | 28:RE:61:ARG:HB3   | 2.06                     | 0.54              |
| 25:YA:825:C:H1'    | 35:YP:55:ARG:HH21  | 1.73                     | 0.54              |
| 36:RQ:12:GLN:HG2   | 36:RQ:73:PRO:HD2   | 1.90                     | 0.54              |
| 29:YF:101:LEU:O    | 29:YF:106:ARG:NH1  | 2.40                     | 0.54              |
| 25:RA:1614:A:H61   | 42:RW:88:ARG:H     | 1.55                     | 0.54              |
| 25:RA:2849:U:O2'   | 25:RA:2868:A:N3    | 2.40                     | 0.54              |
| 45:YZ:27:VAL:HG22  | 45:YZ:29:TYR:HD2   | 1.73                     | 0.54              |
| 25:RA:1330:C:H2'   | 25:RA:1331:A:H8    | 1.72                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:1305:G:N2    | 1:QA:1331:G:H2'    | 2.22                     | 0.54              |
| 1:QA:1227:A:OP1   | 19:QS:80:TYR:OH    | 2.20                     | 0.54              |
| 25:YA:2572:A:N7   | 28:YE:144:ARG:HD2  | 2.22                     | 0.54              |
| 1:QA:1301:U:H2'   | 1:QA:1301:U:O2     | 2.08                     | 0.54              |
| 1:XA:78:G:H1      | 1:XA:92:C:H42      | 1.56                     | 0.54              |
| 1:QA:412:A:C6     | 4:QD:35:ARG:HG2    | 2.43                     | 0.54              |
| 1:XA:1240:U:C4    | 7:XG:32:ARG:HG3    | 2.42                     | 0.54              |
| 49:Y3:59:VAL:HG12 | 49:Y3:60:GLU:H     | 1.72                     | 0.54              |
| 47:Y1:23:LYS:HE3  | 47:Y1:28:GLY:HA3   | 1.88                     | 0.54              |
| 1:QA:1492:A:O2'   | 1:QA:1493:A:N7     | 2.31                     | 0.54              |
| 20:QT:67:ALA:O    | 20:QT:73:HIS:ND1   | 2.40                     | 0.54              |
| 25:RA:2091:U:H5'' | 25:RA:2092:U:H5''  | 1.89                     | 0.54              |
| 27:RD:65:ILE:HD11 | 27:RD:67:PHE:CE2   | 2.43                     | 0.54              |
| 36:YQ:12:GLN:HG2  | 36:YQ:73:PRO:HD2   | 1.88                     | 0.54              |
| 18:XR:62:GLU:HA   | 18:XR:65:ILE:HD11  | 1.90                     | 0.54              |
| 25:YA:1845:G:OP1  | 27:YD:258:LYS:NZ   | 2.37                     | 0.54              |
| 25:RA:78:A:H2'    | 25:RA:79:G:H8      | 1.73                     | 0.54              |
| 5:QE:75:THR:OG1   | 5:QE:76:ILE:N      | 2.40                     | 0.54              |
| 1:QA:642:A:N3     | 8:QH:113:SER:OG    | 2.41                     | 0.54              |
| 35:YP:100:LEU:HB3 | 35:YP:106:LEU:HD13 | 1.88                     | 0.54              |
| 28:RE:79:ARG:NH1  | 28:RE:164:ARG:HH12 | 2.06                     | 0.54              |
| 28:RE:63:LEU:O    | 28:RE:64:LYS:HB2   | 2.06                     | 0.54              |
| 25:YA:6:A:C2      | 25:YA:7:G:C5       | 2.96                     | 0.54              |
| 25:RA:1695:G:C2'  | 25:RA:1696:G:C5'   | 2.86                     | 0.54              |
| 25:RA:2584:U:H2'  | 25:RA:2585:U:H2'   | 1.89                     | 0.54              |
| 25:YA:2105:C:H2'  | 25:YA:2106:G:C8    | 2.41                     | 0.54              |
| 25:RA:2477:C:H2'  | 55:R9:1:MET:HG3    | 1.88                     | 0.54              |
| 1:XA:1237:C:O2'   | 1:XA:1300:G:N2     | 2.38                     | 0.54              |
| 1:XA:452:A:OP1    | 16:XP:43:LYS:NZ    | 2.41                     | 0.54              |
| 41:YV:7:THR:HG23  | 41:YV:22:VAL:HG21  | 1.90                     | 0.54              |
| 45:YZ:10:ARG:NH1  | 45:YZ:26:GLY:O     | 2.41                     | 0.54              |
| 25:RA:2562:U:O2'  | 34:RO:23:ARG:NH1   | 2.40                     | 0.54              |
| 34:RO:97:ARG:HH11 | 34:RO:97:ARG:HG3   | 1.72                     | 0.54              |
| 1:QA:1033:G:O2'   | 1:QA:1034:G:OP1    | 2.23                     | 0.54              |
| 41:YV:35:LEU:O    | 41:YV:37:VAL:HG22  | 2.08                     | 0.54              |
| 4:QD:26:CYS:HA    | 4:QD:31:CYS:HB2    | 1.89                     | 0.54              |
| 27:YD:35:LYS:HZ1  | 27:YD:65:ILE:HA    | 1.72                     | 0.54              |
| 39:YT:24:PRO:HA   | 39:YT:49:VAL:HG13  | 1.90                     | 0.54              |
| 25:RA:2344:U:H6   | 25:RA:2344:U:O5'   | 1.91                     | 0.54              |
| 25:YA:1786:A:H1'  | 25:YA:1938:A:N6    | 2.23                     | 0.54              |
| 1:XA:1308:U:OP1   | 13:XM:98:VAL:N     | 2.30                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:YZ:69:THR:HB    | 45:YZ:88:PHE:HB3   | 1.90                     | 0.54              |
| 31:YH:97:ARG:HB2   | 31:YH:104:GLU:HB2  | 1.90                     | 0.54              |
| 1:QA:1062:U:H2'    | 1:QA:1063:C:C6     | 2.43                     | 0.54              |
| 25:RA:1569:A:H5'   | 27:RD:61:LEU:HD21  | 1.90                     | 0.54              |
| 25:RA:2563:U:H4'   | 34:RO:28:SER:HA    | 1.90                     | 0.54              |
| 25:YA:250:G:H2'    | 25:YA:251:A:C8     | 2.42                     | 0.54              |
| 25:RA:2343:C:H6    | 25:RA:2343:C:H5''  | 1.72                     | 0.54              |
| 35:RP:146:VAL:HG22 | 35:RP:147:LEU:H    | 1.72                     | 0.54              |
| 25:YA:974:G:O2'    | 25:YA:975:G:N7     | 2.35                     | 0.54              |
| 13:XM:46:LYS:O     | 13:XM:48:LEU:N     | 2.40                     | 0.54              |
| 3:XC:60:ALA:O      | 3:XC:63:ASN:ND2    | 2.40                     | 0.54              |
| 1:XA:243:A:H4'     | 1:XA:244:U:O5'     | 2.06                     | 0.54              |
| 4:QD:78:LEU:HD22   | 4:QD:96:LEU:HB3    | 1.90                     | 0.54              |
| 25:YA:2838:G:H1'   | 37:YR:45:ARG:HH12  | 1.73                     | 0.54              |
| 25:RA:39:C:O2      | 29:RF:46:ARG:NH2   | 2.41                     | 0.54              |
| 44:RY:97:ARG:H     | 44:RY:97:ARG:HD3   | 1.72                     | 0.53              |
| 25:RA:1696:G:H2'   | 25:RA:1697:G:O5'   | 2.08                     | 0.53              |
| 40:RU:97:ASP:OD2   | 40:RU:101:ARG:NH2  | 2.41                     | 0.53              |
| 37:RR:33:ARG:HD2   | 51:R5:55:ARG:HD2   | 1.88                     | 0.53              |
| 1:QA:501:C:H2'     | 1:QA:502:G:C8      | 2.42                     | 0.53              |
| 25:RA:2346:A:C2    | 52:R6:25:LYS:HB3   | 2.43                     | 0.53              |
| 1:QA:314:C:O2'     | 1:QA:315:A:H5'     | 2.06                     | 0.53              |
| 1:XA:1302:U:C5     | 13:XM:17:VAL:HG21  | 2.43                     | 0.53              |
| 22:XW:36:U:O4      | 22:XW:37:A:N6      | 2.40                     | 0.53              |
| 25:YA:2059:A:H5'   | 25:YA:2060:A:OP2   | 2.07                     | 0.53              |
| 20:XT:89:ARG:HB2   | 20:XT:104:LEU:HD21 | 1.90                     | 0.53              |
| 38:RS:99:LYS:O     | 38:RS:103:GLU:HG2  | 2.08                     | 0.53              |
| 47:Y1:3:LYS:H      | 47:Y1:61:ARG:HH12  | 1.55                     | 0.53              |
| 29:YF:39:TRP:O     | 29:YF:43:LYS:HG2   | 2.07                     | 0.53              |
| 1:QA:1259:C:N4     | 1:QA:1260:C:O2     | 2.42                     | 0.53              |
| 34:RO:115:VAL:HG13 | 34:RO:121:VAL:HG21 | 1.90                     | 0.53              |
| 25:YA:796:C:H2'    | 25:YA:797:C:C6     | 2.44                     | 0.53              |
| 36:YQ:66:ILE:HD13  | 36:YQ:66:ILE:H     | 1.72                     | 0.53              |
| 24:XY:67:THR:HA    | 24:XY:73:ARG:HD3   | 1.89                     | 0.53              |
| 27:YD:99:ASP:OD2   | 27:YD:101:GLU:N    | 2.32                     | 0.53              |
| 1:XA:1287:A:H2'    | 1:XA:1288:A:C8     | 2.44                     | 0.53              |
| 25:RA:755:C:H2'    | 25:RA:756:C:C6     | 2.44                     | 0.53              |
| 1:XA:976:G:N2      | 1:XA:1363:C:OP2    | 2.23                     | 0.53              |
| 1:QA:1004:A:O2'    | 1:QA:1005:A:O5'    | 2.24                     | 0.53              |
| 7:XG:77:SER:HB2    | 22:XW:32:C:H4'     | 1.90                     | 0.53              |
| 25:YA:2795:G:H21   | 25:YA:2801:A:H62   | 1.56                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:918:A:N3     | 26:RB:80:U:O2'    | 2.41                     | 0.53              |
| 28:RE:3:GLY:HA2    | 28:RE:198:VAL:O   | 2.08                     | 0.53              |
| 18:XR:18:ARG:HG2   | 18:XR:20:ALA:H    | 1.72                     | 0.53              |
| 22:QV:19:G:O6      | 30:RG:83:ARG:NH2  | 2.40                     | 0.53              |
| 25:YA:2291:U:H2'   | 25:YA:2292:C:C6   | 2.44                     | 0.53              |
| 4:XD:150:GLU:HG2   | 4:XD:151:LYS:H    | 1.72                     | 0.53              |
| 25:RA:2306:C:H3'   | 25:RA:2307:G:H5'' | 1.89                     | 0.53              |
| 25:RA:1562:A:H2'   | 25:RA:1563:G:C8   | 2.43                     | 0.53              |
| 4:QD:33:MET:O      | 4:QD:34:GLU:HG2   | 2.08                     | 0.53              |
| 25:YA:2774:C:H2'   | 25:YA:2775:A:O4'  | 2.09                     | 0.53              |
| 25:RA:2786:U:H5''  | 28:RE:66:HIS:HD2  | 1.73                     | 0.53              |
| 25:RA:1250:G:OP2   | 35:RP:21:ARG:NH1  | 2.42                     | 0.53              |
| 40:YU:92:ARG:HG3   | 40:YU:95:LEU:H    | 1.73                     | 0.53              |
| 25:RA:2344:U:OP1   | 52:R6:38:LYS:HD3  | 2.09                     | 0.53              |
| 25:RA:2291:U:O2'   | 25:RA:2374:C:O2   | 2.25                     | 0.53              |
| 25:YA:54:G:O2'     | 53:Y7:35:ARG:HD3  | 2.07                     | 0.53              |
| 25:YA:2870:C:H5''  | 37:YR:65:LEU:HD21 | 1.90                     | 0.53              |
| 35:YP:125:VAL:HG13 | 35:YP:144:GLU:HB3 | 1.89                     | 0.53              |
| 3:QC:22:TRP:CG     | 3:QC:59:ARG:HD2   | 2.44                     | 0.53              |
| 25:YA:78:A:H2'     | 25:YA:79:G:C8     | 2.44                     | 0.53              |
| 3:QC:82:GLU:HG3    | 3:QC:83:ARG:H     | 1.74                     | 0.53              |
| 1:QA:518:C:H4'     | 1:QA:519:C:O5'    | 2.08                     | 0.53              |
| 6:XF:82:ARG:O      | 6:XF:85:VAL:HG23  | 2.08                     | 0.53              |
| 1:XA:757:U:H2'     | 1:XA:758:G:O4'    | 2.09                     | 0.53              |
| 1:QA:1125:U:H2'    | 1:QA:1126:U:H2'   | 1.90                     | 0.53              |
| 7:QG:77:SER:HB2    | 22:QW:32:C:O2'    | 2.08                     | 0.53              |
| 1:XA:960:U:C1'     | 1:XA:961:U:OP2    | 2.57                     | 0.53              |
| 25:RA:2091:U:H1'   | 47:R1:47:GLN:HE21 | 1.73                     | 0.53              |
| 25:RA:2848:G:C8    | 39:RT:97:ALA:HB2  | 2.44                     | 0.53              |
| 25:YA:1598:C:H5'   | 43:YX:36:LYS:HB3  | 1.90                     | 0.53              |
| 1:XA:187:C:H5''    | 20:XT:86:ARG:HG3  | 1.90                     | 0.53              |
| 1:XA:1033:G:O2'    | 1:XA:1034:G:OP1   | 2.25                     | 0.53              |
| 25:RA:775:G:H4'    | 25:RA:776:G:H5'   | 1.89                     | 0.53              |
| 25:RA:250:G:H2'    | 25:RA:251:A:C8    | 2.42                     | 0.53              |
| 25:YA:888:C:H4'    | 25:YA:889:C:H5    | 1.72                     | 0.53              |
| 25:RA:469:G:P      | 29:RF:60:SER:HB3  | 2.48                     | 0.53              |
| 47:Y1:56:GLN:OE1   | 47:Y1:56:GLN:N    | 2.41                     | 0.53              |
| 31:RH:107:VAL:HB   | 31:RH:153:LYS:HG3 | 1.91                     | 0.53              |
| 25:RA:644:A:H4'    | 25:RA:645:C:H5    | 1.74                     | 0.53              |
| 25:YA:2210:G:H3'   | 25:YA:2211:G:C8   | 2.43                     | 0.53              |
| 44:RY:95:LYS:HZ3   | 44:RY:95:LYS:HB2  | 1.74                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:RZ:155:LEU:O    | 45:RZ:156:LYS:CG   | 2.42                     | 0.53              |
| 30:RG:60:LEU:O     | 30:RG:64:THR:HG22  | 2.08                     | 0.53              |
| 25:RA:307:G:N1     | 25:RA:310:A:OP2    | 2.42                     | 0.53              |
| 40:RU:98:LEU:C     | 40:RU:100:VAL:H    | 2.11                     | 0.53              |
| 25:YA:65:C:O2'     | 25:YA:456:C:N3     | 2.31                     | 0.53              |
| 9:XI:2:GLU:H       | 9:XI:20:ARG:HD3    | 1.73                     | 0.53              |
| 1:QA:736:C:H2'     | 1:QA:737:A:C8      | 2.43                     | 0.53              |
| 1:QA:411:A:C8      | 1:QA:413:G:H1'     | 2.43                     | 0.53              |
| 25:RA:1028:A:N3    | 25:RA:2486:G:O2'   | 2.35                     | 0.53              |
| 1:QA:1148:U:H2'    | 1:QA:1149:C:O4'    | 2.09                     | 0.53              |
| 25:YA:1379:A:H4'   | 25:YA:1380:G:OP2   | 2.09                     | 0.53              |
| 25:RA:783:A:O2'    | 25:RA:785:G:OP1    | 2.22                     | 0.53              |
| 47:R1:82:LEU:HD11  | 47:R1:86:SER:HB3   | 1.91                     | 0.53              |
| 1:XA:1187:G:H21    | 14:XN:60:SER:HB3   | 1.72                     | 0.53              |
| 1:QA:444:C:H2'     | 1:QA:445:G:H8      | 1.74                     | 0.53              |
| 18:XR:19:LYS:O     | 18:XR:21:LYS:N     | 2.40                     | 0.53              |
| 37:YR:37:THR:HG22  | 37:YR:39:PRO:HD2   | 1.89                     | 0.53              |
| 42:YW:80:PRO:O     | 42:YW:100:THR:HG22 | 2.08                     | 0.53              |
| 1:XA:928:G:O2'     | 1:XA:1533:C:O2'    | 2.26                     | 0.53              |
| 1:XA:1007:C:H3'    | 1:XA:1008:C:H5''   | 1.91                     | 0.53              |
| 8:QH:86:ILE:HG13   | 8:QH:133:LEU:HD22  | 1.91                     | 0.53              |
| 1:XA:1060:C:C5     | 3:XC:3:ASN:OD1     | 2.62                     | 0.53              |
| 10:XJ:49:VAL:O     | 10:XJ:60:ARG:HB2   | 2.08                     | 0.53              |
| 32:YI:145:VAL:HG13 | 32:YI:145:VAL:O    | 2.09                     | 0.53              |
| 1:QA:716:A:C5      | 1:QA:717:C:C5      | 2.96                     | 0.53              |
| 25:RA:2091:U:H3'   | 25:RA:2092:U:C5'   | 2.38                     | 0.53              |
| 1:QA:1152:A:H5''   | 10:QJ:13:HIS:HD2   | 1.73                     | 0.53              |
| 1:QA:985:C:H2'     | 1:QA:986:A:C8      | 2.44                     | 0.53              |
| 25:YA:582:G:H2'    | 25:YA:583:G:C8     | 2.43                     | 0.53              |
| 28:YE:117:MET:O    | 28:YE:118:LYS:HB2  | 2.08                     | 0.53              |
| 13:QM:11:ARG:O     | 13:QM:13:LYS:N     | 2.41                     | 0.53              |
| 25:RA:1628:G:H2'   | 25:RA:1629:U:C6    | 2.44                     | 0.53              |
| 6:XF:6:VAL:HG13    | 6:XF:90:VAL:HG22   | 1.88                     | 0.53              |
| 1:QA:922:G:H4'     | 5:QE:20:GLN:HA     | 1.90                     | 0.53              |
| 13:QM:46:LYS:O     | 13:QM:48:LEU:N     | 2.42                     | 0.53              |
| 25:YA:997:G:H5''   | 40:YU:58:ARG:HH12  | 1.74                     | 0.53              |
| 52:Y6:28:ARG:HG3   | 52:Y6:30:THR:H     | 1.73                     | 0.53              |
| 25:YA:242:G:C5'    | 54:Y8:62:LEU:HD13  | 2.35                     | 0.53              |
| 27:RD:34:VAL:HG22  | 27:RD:35:LYS:HG3   | 1.89                     | 0.53              |
| 36:YQ:78:PRO:O     | 36:YQ:79:LEU:HG    | 2.08                     | 0.53              |
| 25:RA:637:A:H5''   | 35:RP:117:GLU:HG3  | 1.89                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:382:A:H2'     | 1:XA:383:A:C8      | 2.44                     | 0.53              |
| 1:XA:1060:C:H5''   | 10:XJ:51:ARG:HG2   | 1.91                     | 0.53              |
| 28:RE:62:PRO:O     | 28:RE:63:LEU:C     | 2.47                     | 0.53              |
| 1:QA:1493:A:C2'    | 1:QA:1494:G:H5'    | 2.37                     | 0.53              |
| 45:RZ:118:GLN:HG3  | 45:RZ:174:VAL:H    | 1.73                     | 0.53              |
| 3:QC:164:ARG:NH1   | 3:QC:166:GLU:OE1   | 2.38                     | 0.53              |
| 2:QB:162:ILE:HD11  | 2:QB:184:VAL:HG22  | 1.90                     | 0.53              |
| 19:XS:42:PRO:HG3   | 50:Y4:60:GLN:HE21  | 1.74                     | 0.53              |
| 6:QF:22:GLU:OE1    | 6:QF:84:ASN:ND2    | 2.37                     | 0.53              |
| 25:YA:1109:C:N3    | 25:YA:1110:G:N2    | 2.57                     | 0.53              |
| 25:RA:630:G:N2     | 25:RA:633:A:OP2    | 2.39                     | 0.53              |
| 8:QH:51:VAL:HG11   | 8:QH:60:ARG:HH11   | 1.74                     | 0.53              |
| 1:XA:1325:C:H4'    | 21:XU:17:THR:HG21  | 1.89                     | 0.53              |
| 46:Y0:17:GLN:O     | 46:Y0:19:LYS:NZ    | 2.42                     | 0.53              |
| 25:YA:270(B):A:H5' | 25:YA:270(C):C:OP2 | 2.09                     | 0.53              |
| 54:Y8:14:VAL:HG11  | 54:Y8:22:VAL:HG12  | 1.91                     | 0.53              |
| 3:QC:52:LEU:HD12   | 3:QC:55:VAL:HG22   | 1.90                     | 0.53              |
| 25:RA:1754:C:OP1   | 39:RT:96:ARG:NH1   | 2.42                     | 0.53              |
| 1:QA:1442(A):G:N2  | 25:RA:2863:C:O3'   | 2.41                     | 0.53              |
| 3:XC:180:ALA:HB1   | 3:XC:182:ILE:HG13  | 1.90                     | 0.53              |
| 25:YA:686:G:H5''   | 53:Y7:11:LYS:HE2   | 1.91                     | 0.53              |
| 25:YA:2467:C:O2    | 36:YQ:124:LYS:NZ   | 2.40                     | 0.53              |
| 10:XJ:56:HIS:O     | 10:XJ:58:ASP:N     | 2.41                     | 0.53              |
| 50:R4:10:VAL:O     | 50:R4:25:TYR:HA    | 2.09                     | 0.53              |
| 28:RE:131:ALA:HB1  | 28:RE:135:HIS:HE1  | 1.74                     | 0.53              |
| 31:RH:113:VAL:HG11 | 31:RH:151:ILE:HG21 | 1.91                     | 0.53              |
| 4:QD:57:ARG:HB3    | 4:QD:206:PHE:HB2   | 1.90                     | 0.53              |
| 25:RA:601:C:O2'    | 25:RA:605:C:H5''   | 2.08                     | 0.53              |
| 35:YP:26:GLY:O     | 35:YP:28:GLY:N     | 2.42                     | 0.53              |
| 1:QA:1363(A):A:H4' | 1:QA:1364:U:H5''   | 1.91                     | 0.53              |
| 11:QK:24:SER:OG    | 11:QK:25:TYR:N     | 2.42                     | 0.53              |
| 25:RA:1309:G:H4'   | 53:R7:7:PRO:HB2    | 1.91                     | 0.53              |
| 1:QA:946:A:H2'     | 1:QA:947:G:C8      | 2.44                     | 0.53              |
| 10:QJ:40:LEU:HG    | 10:QJ:41:PRO:HD2   | 1.90                     | 0.53              |
| 4:QD:199:ASN:O     | 4:QD:201:GLN:N     | 2.39                     | 0.53              |
| 34:RO:113:LYS:O    | 34:RO:117:LEU:HB2  | 2.08                     | 0.53              |
| 1:XA:1151:A:H2'    | 1:XA:1152:A:H8     | 1.73                     | 0.53              |
| 36:RQ:80:GLU:HG2   | 46:R0:7:LEU:HD21   | 1.91                     | 0.53              |
| 1:XA:359:U:H2'     | 1:XA:360:A:C8      | 2.44                     | 0.53              |
| 48:R2:47:ASN:O     | 48:R2:49:LYS:N     | 2.36                     | 0.53              |
| 25:YA:2887:U:H2'   | 25:YA:2888:C:C6    | 2.44                     | 0.53              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:RA:2262:U:H2'   | 25:RA:2263:C:C6     | 2.44                     | 0.53              |
| 25:RA:2124:G:H1    | 25:RA:2174:C:H42    | 1.57                     | 0.53              |
| 1:QA:920:U:H2'     | 1:QA:921:U:C6       | 2.43                     | 0.53              |
| 6:XF:62:TRP:CH2    | 6:XF:64:GLN:HB2     | 2.44                     | 0.53              |
| 1:QA:560:U:H4'     | 1:QA:561:U:H5''     | 1.91                     | 0.53              |
| 1:QA:389:A:C6      | 1:QA:390:C:H1'      | 2.44                     | 0.53              |
| 22:XV:9:G:O2'      | 22:XV:10:G:N7       | 2.38                     | 0.53              |
| 25:RA:1571:A:H2'   | 25:RA:1572:A:C8     | 2.44                     | 0.53              |
| 28:RE:37:ARG:N     | 28:RE:46:ALA:O      | 2.37                     | 0.52              |
| 25:RA:1695:G:H2'   | 25:RA:1696:G:C4'    | 2.39                     | 0.52              |
| 25:RA:1695:G:C2'   | 25:RA:1696:G:H5'    | 2.39                     | 0.52              |
| 22:QW:58:A:H1'     | 22:QW:60:U:C5       | 2.44                     | 0.52              |
| 13:XM:4:ILE:HG23   | 13:XM:5:ALA:H       | 1.74                     | 0.52              |
| 13:QM:4:ILE:HA     | 13:QM:57:ARG:HG2    | 1.90                     | 0.52              |
| 25:YA:2469:A:H2    | 25:YA:2481:G:H21    | 1.56                     | 0.52              |
| 48:Y2:46:GLN:HB2   | 48:Y2:49:LYS:HZ1    | 1.74                     | 0.52              |
| 1:QA:411:A:C4      | 1:QA:413:G:H1'      | 2.44                     | 0.52              |
| 13:XM:88:ARG:HG3   | 13:XM:98:VAL:HG13   | 1.91                     | 0.52              |
| 1:QA:530:G:C4      | 23:QX:21:A2M:H2     | 2.44                     | 0.52              |
| 27:RD:148:GLU:HB2  | 27:RD:151:LYS:HD2   | 1.90                     | 0.52              |
| 1:XA:35:G:N3       | 12:XL:118:SER:OG    | 2.42                     | 0.52              |
| 30:RG:53:LEU:HG    | 30:RG:90:LEU:HD21   | 1.90                     | 0.52              |
| 30:RG:55:LYS:HD2   | 30:RG:58:GLN:HE21   | 1.74                     | 0.52              |
| 35:RP:57:THR:CG2   | 35:RP:60:MET:CG     | 2.85                     | 0.52              |
| 22:XV:55:U:O2'     | 22:XV:57:A:N7       | 2.43                     | 0.52              |
| 1:QA:1223:C:P      | 19:QS:78:ARG:HH21   | 2.32                     | 0.52              |
| 19:QS:67:VAL:HG13  | 19:QS:68:GLY:H      | 1.73                     | 0.52              |
| 23:QX:9:G:H4'      | 23:QX:10:G:OP2      | 2.08                     | 0.52              |
| 25:YA:2415:G:H4'   | 35:YP:67:MET:N      | 2.25                     | 0.52              |
| 25:RA:614(A):U:H4' | 25:RA:614(B):G:H5'' | 1.91                     | 0.52              |
| 25:YA:1754:C:OP1   | 39:YT:96:ARG:NH1    | 2.42                     | 0.52              |
| 25:RA:1562:A:H2'   | 25:RA:1563:G:H8     | 1.74                     | 0.52              |
| 27:RD:228:PRO:HD3  | 27:RD:235:GLY:CA    | 2.40                     | 0.52              |
| 1:XA:689:C:H2'     | 1:XA:690:G:O4'      | 2.09                     | 0.52              |
| 45:YZ:94:GLU:HG3   | 45:YZ:129:SER:HB3   | 1.89                     | 0.52              |
| 25:RA:1273:U:O2'   | 25:RA:1275:A:OP1    | 2.27                     | 0.52              |
| 21:QU:12:LYS:HB3   | 21:QU:22:ARG:HD2    | 1.91                     | 0.52              |
| 25:YA:764:A:O4'    | 27:YD:213:ARG:HG3   | 2.09                     | 0.52              |
| 35:RP:12:ALA:C     | 35:RP:14:LYS:H      | 2.12                     | 0.52              |
| 1:XA:960:U:O2      | 1:XA:960:U:C2'      | 2.54                     | 0.52              |
| 25:YA:1190:G:OP1   | 35:YP:30:THR:OG1    | 2.23                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:422:C:HO2'   | 1:QA:423:G:N2      | 2.07                     | 0.52              |
| 1:QA:437:U:H5'    | 4:QD:155:LEU:HD21  | 1.91                     | 0.52              |
| 25:YA:859:G:N2    | 25:YA:917:A:OP2    | 2.43                     | 0.52              |
| 25:YA:587:C:OP2   | 35:YP:21:ARG:NH2   | 2.42                     | 0.52              |
| 1:XA:707:C:H2'    | 1:XA:708:C:C6      | 2.45                     | 0.52              |
| 25:RA:2836:U:H2'  | 25:RA:2837:G:C8    | 2.44                     | 0.52              |
| 1:XA:1077:G:N2    | 1:XA:1080:A:OP2    | 2.39                     | 0.52              |
| 25:YA:2393:A:H2'  | 25:YA:2394:C:O4'   | 2.10                     | 0.52              |
| 1:QA:353:A:C8     | 1:QA:353:A:C5'     | 2.86                     | 0.52              |
| 41:YV:2:PHE:HE1   | 41:YV:4:ILE:HD13   | 1.74                     | 0.52              |
| 1:QA:350:G:C8     | 1:QA:350:G:H5'     | 2.43                     | 0.52              |
| 47:Y1:85:LEU:HD22 | 47:Y1:88:LYS:HG3   | 1.90                     | 0.52              |
| 1:QA:716:A:C6     | 1:QA:717:C:C4      | 2.98                     | 0.52              |
| 45:RZ:91:LEU:HD12 | 45:RZ:130:PRO:HB3  | 1.90                     | 0.52              |
| 1:QA:1034:G:H2'   | 1:QA:1035:A:C8     | 2.44                     | 0.52              |
| 8:QH:41:ARG:NH2   | 8:QH:123:GLU:OE2   | 2.41                     | 0.52              |
| 29:RF:66:PRO:O    | 29:RF:67:GLN:HB3   | 2.10                     | 0.52              |
| 4:XD:22:LYS:HB2   | 4:XD:26:CYS:HB2    | 1.90                     | 0.52              |
| 29:RF:2:LYS:HG3   | 29:RF:24:LEU:HD12  | 1.92                     | 0.52              |
| 25:RA:2207:G:H2'  | 25:RA:2207:G:N3    | 2.24                     | 0.52              |
| 25:RA:686:G:H21   | 25:RA:788:A:H61    | 1.58                     | 0.52              |
| 25:RA:2746:U:H5'' | 31:RH:138:LYS:HE3  | 1.92                     | 0.52              |
| 1:XA:736:C:H2'    | 1:XA:737:A:C8      | 2.45                     | 0.52              |
| 31:YH:97:ARG:N    | 31:YH:104:GLU:O    | 2.40                     | 0.52              |
| 8:QH:34:GLU:OE1   | 8:QH:37:ARG:NH1    | 2.43                     | 0.52              |
| 49:R3:7:LYS:HB2   | 49:R3:34:GLU:HG2   | 1.90                     | 0.52              |
| 25:YA:2420:C:H41  | 54:Y8:31:HIS:HA    | 1.75                     | 0.52              |
| 25:RA:2774:C:H2'  | 25:RA:2775:A:O4'   | 2.09                     | 0.52              |
| 31:RH:10:PRO:O    | 31:RH:11:VAL:HG12  | 2.08                     | 0.52              |
| 28:RE:63:LEU:O    | 28:RE:64:LYS:CB    | 2.57                     | 0.52              |
| 25:RA:674:G:O2'   | 29:RF:74:ARG:HG3   | 2.10                     | 0.52              |
| 45:RZ:157:LEU:HB3 | 45:RZ:161:VAL:CG1  | 2.33                     | 0.52              |
| 52:Y6:28:ARG:HD2  | 52:Y6:29:ASN:CB    | 2.34                     | 0.52              |
| 25:YA:1049:C:N4   | 25:YA:2751:G:O6    | 2.43                     | 0.52              |
| 25:YA:2646:C:OP2  | 25:YA:2732:G:O2'   | 2.23                     | 0.52              |
| 25:RA:2091:U:O2'  | 47:R1:47:GLN:CG    | 2.58                     | 0.52              |
| 25:RA:708:C:H5'   | 25:RA:709:U:OP2    | 2.10                     | 0.52              |
| 25:YA:2579:C:H4'  | 28:YE:134:ILE:HG21 | 1.92                     | 0.52              |
| 2:QB:73:THR:HG21  | 2:QB:97:TRP:HB2    | 1.91                     | 0.52              |
| 40:YU:28:ARG:NH1  | 40:YU:38:THR:OG1   | 2.36                     | 0.52              |
| 25:YA:2502:G:H5'' | 25:YA:2503:A:H5''  | 1.92                     | 0.52              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 25:YA:1889:A:N1   | 25:YA:2234:G:H1'    | 2.24                     | 0.52              |
| 8:XH:29:SER:HB3   | 8:XH:32:LYS:HG3     | 1.91                     | 0.52              |
| 25:YA:2836:U:H2'  | 25:YA:2837:G:C8     | 2.45                     | 0.52              |
| 1:QA:103:C:P      | 20:QT:17:ARG:HH21   | 2.33                     | 0.52              |
| 25:YA:1217:C:OP1  | 40:YU:15:LYS:HE3    | 2.09                     | 0.52              |
| 54:Y8:40:GLU:H    | 54:Y8:43:GLN:HG3    | 1.75                     | 0.52              |
| 44:YY:95:LYS:HA   | 44:YY:101:LYS:HB2   | 1.91                     | 0.52              |
| 45:RZ:156:LYS:CA  | 45:RZ:158:PRO:HD3   | 2.40                     | 0.52              |
| 38:YS:67:ARG:O    | 38:YS:71:ARG:HG3    | 2.09                     | 0.52              |
| 1:XA:1001:A:H3'   | 1:XA:1001(A):G:H5'' | 1.91                     | 0.52              |
| 25:RA:2015:A:H1'  | 51:R5:2:ALA:HA      | 1.90                     | 0.52              |
| 13:XM:19:LEU:HD21 | 13:XM:56:LEU:HD11   | 1.91                     | 0.52              |
| 22:QV:1:C:O2      | 22:QV:1:C:H2'       | 2.08                     | 0.52              |
| 27:YD:4:LYS:HE3   | 27:YD:20:ASP:HA     | 1.91                     | 0.52              |
| 1:QA:1051:C:H2'   | 1:QA:1052:U:C6      | 2.45                     | 0.52              |
| 1:XA:403:C:H2'    | 1:XA:404:U:H6       | 1.74                     | 0.52              |
| 30:RG:118:ARG:HB3 | 30:RG:181:ARG:HG3   | 1.91                     | 0.52              |
| 15:QO:64:ARG:HH11 | 15:QO:68:ARG:HH21   | 1.58                     | 0.52              |
| 25:RA:1988:C:H2'  | 25:RA:1989:G:H8     | 1.75                     | 0.52              |
| 25:YA:1790:C:H5'' | 25:YA:1791:A:OP1    | 2.10                     | 0.52              |
| 1:XA:1166:G:N2    | 1:XA:1170:A:OP2     | 2.43                     | 0.52              |
| 47:R1:56:GLN:OE1  | 47:R1:56:GLN:N      | 2.43                     | 0.52              |
| 9:QI:45:ALA:O     | 9:QI:78:LYS:NZ      | 2.42                     | 0.52              |
| 25:RA:2037:G:H2'  | 25:RA:2038:G:C8     | 2.45                     | 0.52              |
| 1:XA:1293:G:H2'   | 1:XA:1294:G:C8      | 2.44                     | 0.52              |
| 25:RA:2789:C:O2   | 25:RA:2894:G:N2     | 2.39                     | 0.52              |
| 33:RN:14:VAL:HA   | 33:RN:135:PRO:HD2   | 1.92                     | 0.52              |
| 32:RI:129:THR:HA  | 32:RI:137:PRO:HA    | 1.92                     | 0.52              |
| 44:RY:99:CYS:SG   | 44:RY:100:ALA:N     | 2.83                     | 0.52              |
| 35:YP:63:PRO:HD2  | 54:Y8:30:ARG:HH21   | 1.75                     | 0.52              |
| 25:YA:389:G:H1    | 35:YP:71:VAL:HG12   | 1.75                     | 0.52              |
| 25:RA:1021:A:C3'  | 25:RA:1021:A:C8     | 2.93                     | 0.52              |
| 25:YA:910:A:N1    | 25:YA:2277:G:H1'    | 2.25                     | 0.52              |
| 1:QA:1301:U:C4    | 1:QA:1303:C:C6      | 2.98                     | 0.52              |
| 2:QB:97:TRP:HZ2   | 2:QB:102:LEU:HD13   | 1.74                     | 0.52              |
| 25:YA:1027:A:C2   | 25:YA:2488:A:H5'    | 2.44                     | 0.52              |
| 16:QP:18:ARG:HD3  | 16:QP:35:LYS:HD2    | 1.92                     | 0.52              |
| 25:RA:2097:C:H42  | 25:RA:2192:G:H1     | 1.58                     | 0.52              |
| 25:RA:2558:C:H2'  | 25:RA:2559:C:H6     | 1.75                     | 0.52              |
| 1:XA:714:G:H2'    | 1:XA:715:A:C8       | 2.45                     | 0.52              |
| 25:YA:2734:A:H5'  | 25:YA:2735:G:OP2    | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RA:2572:A:C8   | 28:RE:144:ARG:HD2 | 2.45                     | 0.52              |
| 10:XJ:44:VAL:HG22 | 10:XJ:66:ARG:HG2  | 1.92                     | 0.52              |
| 1:XA:1117:G:H4'   | 9:XI:104:ARG:HD2  | 1.91                     | 0.52              |
| 1:XA:563:A:H2'    | 1:XA:567:G:C8     | 2.45                     | 0.52              |
| 31:RH:10:PRO:O    | 31:RH:11:VAL:HG13 | 2.10                     | 0.52              |
| 1:XA:1493:A:N6    | 25:YA:1913:A:H1'  | 2.24                     | 0.52              |
| 33:YN:34:LEU:O    | 33:YN:49:GLY:HA3  | 2.10                     | 0.52              |
| 25:YA:443:A:H1'   | 25:YA:1201:C:O4'  | 2.09                     | 0.52              |
| 30:RG:47:LYS:HD3  | 30:RG:81:LYS:HB2  | 1.91                     | 0.52              |
| 32:YI:27:ARG:HD2  | 47:Y1:71:TYR:CE1  | 2.44                     | 0.52              |
| 55:R9:9:ARG:NH1   | 55:R9:14:CYS:O    | 2.42                     | 0.52              |
| 25:RA:1800:C:OP2  | 27:RD:183:ARG:NH2 | 2.43                     | 0.52              |
| 2:QB:118:LEU:HB3  | 2:QB:142:LEU:HD12 | 1.92                     | 0.52              |
| 1:XA:1411:C:H2'   | 1:XA:1412:C:C6    | 2.45                     | 0.52              |
| 1:XA:413:G:H21    | 1:XA:428:G:H1'    | 1.75                     | 0.52              |
| 1:XA:545:C:OP2    | 4:XD:62:GLN:NE2   | 2.42                     | 0.52              |
| 3:QC:95:THR:HG22  | 3:QC:97:LYS:H     | 1.75                     | 0.52              |
| 19:QS:16:LEU:HD11 | 19:QS:41:VAL:HG11 | 1.90                     | 0.52              |
| 40:RU:81:HIS:HD2  | 40:RU:84:LYS:HD3  | 1.75                     | 0.52              |
| 1:XA:250:A:H4'    | 1:XA:251:G:O5'    | 2.10                     | 0.52              |
| 43:YX:3:THR:HA    | 43:YX:6:ASP:OD2   | 2.10                     | 0.52              |
| 45:RZ:151:HIS:O   | 45:RZ:151:HIS:ND1 | 2.43                     | 0.52              |
| 17:QQ:66:SER:O    | 17:QQ:70:ARG:NH1  | 2.43                     | 0.52              |
| 25:RA:1903:G:OP2  | 27:RD:241:PRO:HB2 | 2.10                     | 0.52              |
| 41:RV:4:ILE:HG22  | 41:RV:39:LEU:HD13 | 1.92                     | 0.52              |
| 25:RA:1254:A:H5'  | 25:RA:1255:U:C5'  | 2.39                     | 0.52              |
| 9:XI:17:VAL:HG11  | 9:XI:81:ILE:HA    | 1.92                     | 0.52              |
| 27:YD:8:PRO:HB3   | 27:YD:14:ARG:HB2  | 1.92                     | 0.52              |
| 1:XA:1412:C:H2'   | 1:XA:1413:A:C8    | 2.45                     | 0.52              |
| 25:YA:1568:G:H4'  | 27:YD:59:LYS:HB3  | 1.92                     | 0.52              |
| 48:Y2:24:LEU:HD13 | 48:Y2:60:LEU:HD21 | 1.92                     | 0.52              |
| 1:QA:243:A:H4'    | 1:QA:244:U:O5'    | 2.08                     | 0.52              |
| 28:RE:7:VAL:HG11  | 39:RT:1:MET:HE1   | 1.92                     | 0.52              |
| 1:QA:482:A:H5'    | 1:QA:483:C:OP2    | 2.10                     | 0.52              |
| 25:RA:923:C:H2'   | 25:RA:924:C:H6    | 1.74                     | 0.52              |
| 25:YA:2591:C:H2'  | 25:YA:2592:G:C8   | 2.45                     | 0.52              |
| 41:YV:87:HIS:NE2  | 41:YV:89:GLN:OE1  | 2.33                     | 0.51              |
| 28:RE:32:PRO:HD2  | 28:RE:50:GLY:O    | 2.11                     | 0.51              |
| 25:YA:2306:C:N4   | 25:YA:2307:G:O6   | 2.44                     | 0.51              |
| 24:XY:26:ASP:OD1  | 24:XY:69:ARG:NE   | 2.41                     | 0.51              |
| 36:RQ:64:ILE:HD13 | 36:RQ:64:ILE:H    | 1.74                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:Y5:6:VAL:O     | 51:Y5:7:PRO:C      | 2.47                     | 0.51              |
| 25:RA:1329:U:H5'' | 25:RA:1330:C:C5    | 2.45                     | 0.51              |
| 1:QA:1288:A:H2'   | 1:QA:1289:A:H8     | 1.75                     | 0.51              |
| 1:QA:1498:U:O2'   | 1:QA:1499:A:OP2    | 2.23                     | 0.51              |
| 1:QA:805:C:H2'    | 1:QA:806:C:H6      | 1.74                     | 0.51              |
| 1:XA:119:A:H4'    | 1:XA:120:A:C8      | 2.45                     | 0.51              |
| 25:YA:2690:C:OP2  | 37:YR:17:ARG:NH1   | 2.39                     | 0.51              |
| 1:XA:126:G:OP1    | 1:XA:605:U:O2'     | 2.26                     | 0.51              |
| 28:YE:24:THR:HG21 | 28:YE:188:VAL:HG12 | 1.92                     | 0.51              |
| 25:RA:2469:A:O2'  | 36:RQ:56:ARG:HG2   | 2.10                     | 0.51              |
| 27:YD:76:PRO:HG2  | 27:YD:98:VAL:HG21  | 1.92                     | 0.51              |
| 3:XC:20:SER:OG    | 3:XC:40:ARG:NH2    | 2.40                     | 0.51              |
| 25:YA:631:A:OP2   | 54:Y8:47:LYS:NZ    | 2.43                     | 0.51              |
| 23:XX:12:A:H2'    | 23:XX:13:A:C8      | 2.45                     | 0.51              |
| 1:XA:769:G:H4'    | 1:XA:1513:A:H4'    | 1.91                     | 0.51              |
| 45:YZ:5:LEU:HD21  | 45:YZ:44:PHE:HA    | 1.92                     | 0.51              |
| 5:XE:33:VAL:HG21  | 5:XE:109:ILE:HG12  | 1.93                     | 0.51              |
| 25:YA:1028:A:N3   | 25:YA:2486:G:O2'   | 2.27                     | 0.51              |
| 37:YR:78:LYS:O    | 37:YR:82:GLU:HB3   | 2.10                     | 0.51              |
| 2:QB:69:LEU:HD23  | 2:QB:91:PRO:HB2    | 1.92                     | 0.51              |
| 1:QA:708:C:H2'    | 1:QA:709:G:H8      | 1.75                     | 0.51              |
| 13:QM:88:ARG:HG3  | 13:QM:98:VAL:HG13  | 1.92                     | 0.51              |
| 26:RB:32:C:O2     | 26:RB:50:G:N2      | 2.28                     | 0.51              |
| 1:XA:67:C:H2'     | 1:XA:68:G:C8       | 2.45                     | 0.51              |
| 52:Y6:28:ARG:CG   | 52:Y6:30:THR:H     | 2.23                     | 0.51              |
| 54:Y8:60:LEU:O    | 54:Y8:62:LEU:N     | 2.43                     | 0.51              |
| 25:YA:1171:G:O2'  | 25:YA:1173:G:O5'   | 2.28                     | 0.51              |
| 1:QA:1068:G:H8    | 1:QA:1068:G:OP2    | 1.92                     | 0.51              |
| 1:XA:1328:C:OP1   | 21:XU:21:TYR:OH    | 2.22                     | 0.51              |
| 9:XI:2:GLU:H      | 9:XI:20:ARG:HH11   | 1.57                     | 0.51              |
| 27:YD:99:ASP:OD2  | 27:YD:101:GLU:CB   | 2.59                     | 0.51              |
| 25:RA:2659:G:N2   | 25:RA:2662:A:OP2   | 2.43                     | 0.51              |
| 5:XE:48:ALA:HB2   | 5:XE:57:LYS:HD3    | 1.91                     | 0.51              |
| 25:YA:2162:G:O2'  | 25:YA:2173:A:OP2   | 2.25                     | 0.51              |
| 33:RN:125:GLY:HA3 | 33:RN:126:PRO:O    | 2.10                     | 0.51              |
| 25:RA:2111:C:C2   | 25:RA:2118:U:H1'   | 2.45                     | 0.51              |
| 1:QA:1001(A):G:N1 | 1:QA:1039:C:N3     | 2.55                     | 0.51              |
| 45:RZ:149:SER:OG  | 45:RZ:150:LEU:N    | 2.42                     | 0.51              |
| 19:XS:67:VAL:HG21 | 50:Y4:59:PHE:CB    | 2.32                     | 0.51              |
| 23:QX:14:A:H2'    | 23:QX:15:A:H5'     | 1.92                     | 0.51              |
| 25:YA:2343:C:H5'' | 25:YA:2343:C:C6    | 2.42                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:YF:132:VAL:C    | 29:YF:134:GLY:H    | 2.13                     | 0.51              |
| 25:RA:2822:G:H2'   | 25:RA:2823:A:H5''  | 1.92                     | 0.51              |
| 28:YE:66:HIS:C     | 28:YE:68:ALA:H     | 2.14                     | 0.51              |
| 43:RX:63:LYS:HA    | 43:RX:72:LYS:HA    | 1.92                     | 0.51              |
| 1:QA:250:A:H5'     | 1:QA:252:U:O4'     | 2.10                     | 0.51              |
| 25:RA:877:U:H2'    | 25:RA:878:A:H5''   | 1.91                     | 0.51              |
| 1:XA:77:G:O6       | 1:XA:92:C:N4       | 2.43                     | 0.51              |
| 25:RA:1865:G:H5'   | 25:RA:1866:C:OP2   | 2.10                     | 0.51              |
| 30:YG:151:ALA:HB3  | 30:YG:153:ARG:NH1  | 2.25                     | 0.51              |
| 30:RG:15:VAL:HG21  | 30:RG:176:LEU:HD23 | 1.93                     | 0.51              |
| 25:RA:1504:C:H2'   | 25:RA:1505:C:H5''  | 1.92                     | 0.51              |
| 25:RA:1062:G:H2'   | 25:RA:1063:G:H8    | 1.75                     | 0.51              |
| 20:QT:40:ALA:HB2   | 20:QT:55:ILE:HG22  | 1.93                     | 0.51              |
| 25:YA:270(F):U:H2' | 25:YA:270(G):C:C6  | 2.45                     | 0.51              |
| 25:RA:2748:A:H2'   | 25:RA:2749:A:O4'   | 2.10                     | 0.51              |
| 25:YA:2393:A:H4'   | 35:YP:62:LEU:N     | 2.26                     | 0.51              |
| 52:Y6:28:ARG:CB    | 52:Y6:30:THR:H     | 2.22                     | 0.51              |
| 25:YA:857:C:H5''   | 46:Y0:77:ARG:NH2   | 2.25                     | 0.51              |
| 1:QA:975:A:H5''    | 1:QA:976:G:H5'     | 1.92                     | 0.51              |
| 1:XA:1314:C:H2'    | 1:XA:1315:U:H6     | 1.73                     | 0.51              |
| 1:QA:404:U:H2'     | 1:QA:405:U:C6      | 2.46                     | 0.51              |
| 37:RR:38:VAL:HG22  | 37:RR:112:ALA:HB2  | 1.92                     | 0.51              |
| 49:R3:59:VAL:HG12  | 49:R3:60:GLU:H     | 1.75                     | 0.51              |
| 25:RA:272(J):C:H3' | 25:RA:274:G:H5''   | 1.92                     | 0.51              |
| 1:XA:811:C:O2'     | 1:XA:901:A:N1      | 2.40                     | 0.51              |
| 25:RA:1795:C:O2    | 27:RD:255:LYS:HE3  | 2.11                     | 0.51              |
| 2:QB:51:LEU:HD23   | 2:QB:201:ILE:HD12  | 1.93                     | 0.51              |
| 41:RV:71:LEU:HD11  | 41:RV:83:ARG:NE    | 2.25                     | 0.51              |
| 9:XI:17:VAL:HG22   | 9:XI:63:ILE:HG12   | 1.92                     | 0.51              |
| 12:XL:27:LEU:HD11  | 12:XL:85:ILE:HG22  | 1.93                     | 0.51              |
| 1:XA:674:G:H2'     | 1:XA:675:A:H8      | 1.76                     | 0.51              |
| 25:RA:709:U:H3     | 25:RA:722:A:H61    | 1.58                     | 0.51              |
| 31:RH:137:ASP:OD1  | 31:RH:138:LYS:N    | 2.39                     | 0.51              |
| 4:QD:33:MET:HE3    | 4:QD:37:PRO:HA     | 1.93                     | 0.51              |
| 31:YH:33:LEU:HD21  | 31:YH:140:LYS:HE2  | 1.92                     | 0.51              |
| 28:RE:119:ARG:HG2  | 28:RE:160:TYR:HB2  | 1.93                     | 0.51              |
| 25:RA:1278:A:OP1   | 37:RR:36:THR:HG22  | 2.11                     | 0.51              |
| 25:RA:380:U:O3'    | 47:R1:16:ASN:HB2   | 2.10                     | 0.51              |
| 25:YA:1982:C:O2    | 25:YA:1982:C:H2'   | 2.10                     | 0.51              |
| 39:RT:26:ASP:O     | 39:RT:49:VAL:HG12  | 2.10                     | 0.51              |
| 25:YA:990:A:C6     | 25:YA:1186:G:H1'   | 2.46                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:373:U:C2     | 25:RA:374:A:C8     | 2.99                     | 0.51              |
| 35:YP:19:VAL:HG13  | 35:YP:21:ARG:H     | 1.76                     | 0.51              |
| 20:XT:48:LYS:HB3   | 20:XT:51:GLU:HG3   | 1.93                     | 0.51              |
| 25:RA:363(F):A:H1' | 25:RA:364:C:H5     | 1.75                     | 0.51              |
| 2:QB:9:GLU:O       | 2:QB:12:GLU:HG3    | 2.10                     | 0.51              |
| 3:QC:150:LYS:HE2   | 3:QC:152:ILE:HD11  | 1.92                     | 0.51              |
| 1:XA:532:A:N6      | 3:XC:193:TYR:HB3   | 2.25                     | 0.51              |
| 28:YE:101:ARG:O    | 28:YE:201:THR:OG1  | 2.29                     | 0.51              |
| 1:XA:45:U:H2'      | 1:XA:46:G:C8       | 2.45                     | 0.51              |
| 30:YG:60:LEU:O     | 30:YG:64:THR:HG22  | 2.10                     | 0.51              |
| 1:QA:278:G:N2      | 17:QQ:95:TYR:HB3   | 2.25                     | 0.51              |
| 12:QL:59:ARG:HA    | 12:QL:65:GLU:HA    | 1.91                     | 0.51              |
| 1:XA:1499:A:H1'    | 1:XA:1520:G:H5'    | 1.93                     | 0.51              |
| 25:YA:1239:G:H2'   | 25:YA:1240:U:O4'   | 2.11                     | 0.51              |
| 39:RT:54:ARG:HA    | 39:RT:59:THR:HB    | 1.92                     | 0.51              |
| 1:QA:674:G:H2'     | 1:QA:675:A:C8      | 2.46                     | 0.51              |
| 25:YA:1007:C:H5''  | 33:YN:35:ARG:HH11  | 1.75                     | 0.51              |
| 21:XU:12:LYS:HG2   | 21:XU:22:ARG:HB3   | 1.92                     | 0.51              |
| 54:Y8:31:HIS:CG    | 54:Y8:32:LEU:H     | 2.27                     | 0.51              |
| 47:R1:44:PRO:O     | 47:R1:46:LEU:N     | 2.43                     | 0.51              |
| 25:YA:1488:G:H5'   | 25:YA:1489:U:OP2   | 2.11                     | 0.51              |
| 1:XA:592:G:H2'     | 1:XA:593:G:H8      | 1.74                     | 0.51              |
| 2:XB:72:GLY:HA3    | 2:XB:81:VAL:HG21   | 1.93                     | 0.51              |
| 25:RA:2529:G:N3    | 25:RA:2529:G:H5''  | 2.26                     | 0.51              |
| 25:RA:547:A:H2'    | 25:RA:548:A:C8     | 2.46                     | 0.51              |
| 1:XA:375:U:O2'     | 16:XP:28:ARG:HD2   | 2.10                     | 0.51              |
| 1:QA:612:C:O2      | 1:QA:629:G:N2      | 2.44                     | 0.51              |
| 37:YR:97:VAL:HG22  | 37:YR:114:VAL:HG22 | 1.93                     | 0.51              |
| 30:YG:11:TYR:HA    | 30:YG:15:VAL:HB    | 1.92                     | 0.51              |
| 42:YW:78:GLU:OE1   | 42:YW:99:ARG:NH1   | 2.41                     | 0.51              |
| 25:YA:1681:G:H8    | 25:YA:1681:G:OP2   | 1.94                     | 0.51              |
| 54:Y8:33:ASN:HB2   | 54:Y8:36:LYS:HD3   | 1.92                     | 0.51              |
| 25:RA:479:A:HO2'   | 25:RA:481:G:H8     | 1.59                     | 0.51              |
| 32:RI:77:LEU:HA    | 32:RI:140:LEU:HD12 | 1.92                     | 0.51              |
| 45:RZ:157:LEU:N    | 45:RZ:158:PRO:CD   | 2.74                     | 0.51              |
| 25:YA:987:G:O2'    | 25:YA:988:A:H5'    | 2.11                     | 0.51              |
| 25:YA:2343:C:C5'   | 25:YA:2343:C:C6    | 2.85                     | 0.51              |
| 1:QA:1323:G:H2'    | 1:QA:1324:A:C8     | 2.46                     | 0.51              |
| 25:RA:659:C:H2'    | 25:RA:660:G:H8     | 1.74                     | 0.51              |
| 1:XA:1280:A:H1'    | 10:XJ:41:PRO:HG3   | 1.91                     | 0.51              |
| 1:QA:1314:C:OP2    | 19:QS:6:LYS:HD2    | 2.11                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:YB:24:G:O6     | 26:YB:56:G:O2'     | 2.29                     | 0.51              |
| 1:QA:404:U:H5'    | 4:QD:122:ARG:HD2   | 1.93                     | 0.51              |
| 8:QH:20:TYR:CE2   | 8:QH:75:ARG:HB3    | 2.46                     | 0.51              |
| 25:RA:352:G:O2'   | 25:RA:353:G:OP1    | 2.26                     | 0.51              |
| 25:YA:582:G:H2'   | 25:YA:583:G:H8     | 1.76                     | 0.51              |
| 25:YA:297:C:H5''  | 44:YY:85:VAL:HG11  | 1.92                     | 0.51              |
| 25:YA:1030:G:OP2  | 36:YQ:128:LYS:HE3  | 2.11                     | 0.51              |
| 1:QA:1106:G:H5''  | 3:QC:172:ARG:HG2   | 1.93                     | 0.51              |
| 25:YA:1766:U:H2'  | 25:YA:1767:C:H6    | 1.75                     | 0.51              |
| 25:RA:411:G:OP2   | 25:RA:2406:U:O2'   | 2.28                     | 0.51              |
| 1:QA:258:G:H2'    | 1:QA:259:G:H8      | 1.75                     | 0.51              |
| 42:YW:25:ARG:NH2  | 42:YW:74:ALA:O     | 2.44                     | 0.51              |
| 49:Y3:6:VAL:HG13  | 49:Y3:54:VAL:HG11  | 1.93                     | 0.51              |
| 1:XA:646:U:H2'    | 1:XA:647:C:C6      | 2.46                     | 0.51              |
| 22:XV:23:C:H2'    | 22:XV:24:U:C6      | 2.45                     | 0.51              |
| 36:YQ:115:MET:HG3 | 36:YQ:131:ILE:HG21 | 1.91                     | 0.51              |
| 1:QA:1347:G:H4'   | 1:QA:1348:U:C6     | 2.46                     | 0.51              |
| 1:XA:960:U:OP1    | 24:XY:8:LYS:CE     | 2.59                     | 0.51              |
| 40:RU:95:LEU:C    | 40:RU:97:ASP:H     | 2.14                     | 0.51              |
| 1:QA:329:A:C5     | 1:QA:332:G:C6      | 2.99                     | 0.51              |
| 51:Y5:2:ALA:O     | 51:Y5:3:LYS:HD2    | 2.10                     | 0.51              |
| 44:RY:69:ALA:O    | 44:RY:72:VAL:HG22  | 2.11                     | 0.51              |
| 26:YB:56:G:H5'    | 30:YG:27:ASN:HD21  | 1.75                     | 0.51              |
| 20:QT:10:LEU:HD22 | 20:QT:11:SER:H     | 1.74                     | 0.51              |
| 25:RA:1570:A:H2'  | 25:RA:1571:A:C8    | 2.46                     | 0.51              |
| 1:XA:115:G:H4'    | 1:XA:116:A:O5'     | 2.11                     | 0.51              |
| 1:QA:1325:C:H4'   | 21:QU:17:THR:HG21  | 1.92                     | 0.51              |
| 52:R6:12:GLU:HB2  | 52:R6:22:ALA:HB3   | 1.93                     | 0.51              |
| 16:QP:53:VAL:HG12 | 16:QP:79:VAL:HG22  | 1.92                     | 0.51              |
| 22:XW:53:G:H1     | 22:XW:61:C:H42     | 1.57                     | 0.51              |
| 32:RI:101:LEU:H   | 32:RI:101:LEU:HD23 | 1.76                     | 0.51              |
| 6:XF:76:ALA:O     | 6:XF:80:ARG:HG3    | 2.11                     | 0.51              |
| 30:RG:131:TYR:HB3 | 30:RG:159:VAL:HG13 | 1.92                     | 0.51              |
| 1:XA:392:G:H2'    | 1:XA:393:A:C8      | 2.46                     | 0.51              |
| 9:XI:37:PHE:HE2   | 9:XI:70:LYS:HG3    | 1.76                     | 0.51              |
| 25:YA:2219:G:OP1  | 27:YD:172:TYR:OH   | 2.22                     | 0.51              |
| 28:RE:33:VAL:HG12 | 28:RE:90:THR:H     | 1.75                     | 0.50              |
| 41:RV:40:LEU:HD21 | 41:RV:47:VAL:HB    | 1.93                     | 0.50              |
| 4:QD:9:CYS:HA     | 4:QD:12:CYS:HB2    | 1.93                     | 0.50              |
| 10:QJ:49:VAL:O    | 10:QJ:60:ARG:HB2   | 2.11                     | 0.50              |
| 31:RH:126:PRO:HB2 | 31:RH:127:GLU:HA   | 1.94                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:YQ:19:GLY:H    | 36:YQ:98:LYS:NZ    | 2.08                     | 0.50              |
| 25:YA:2208:U:H4'  | 27:YD:151:LYS:HG2  | 1.92                     | 0.50              |
| 25:YA:2572:A:C8   | 28:YE:144:ARG:HD2  | 2.46                     | 0.50              |
| 26:RB:64:C:H2'    | 26:RB:65:C:H6      | 1.76                     | 0.50              |
| 25:RA:2572:A:N7   | 28:RE:144:ARG:HD2  | 2.26                     | 0.50              |
| 25:YA:1578:U:H2'  | 25:YA:1579:A:H5'   | 1.93                     | 0.50              |
| 7:QG:20:ASP:OD2   | 7:QG:23:VAL:N      | 2.45                     | 0.50              |
| 39:RT:62:THR:HG22 | 39:RT:75:ILE:HG23  | 1.92                     | 0.50              |
| 22:XW:21:A:H61    | 22:XW:46:G:H2'     | 1.75                     | 0.50              |
| 25:RA:1341:U:H3'  | 25:RA:1397:U:O2    | 2.11                     | 0.50              |
| 47:Y1:94:LEU:H    | 47:Y1:94:LEU:HD23  | 1.76                     | 0.50              |
| 25:YA:2584:U:O2   | 25:YA:2584:U:O5'   | 2.30                     | 0.50              |
| 5:QE:147:ASP:OD2  | 5:QE:147:ASP:N     | 2.24                     | 0.50              |
| 1:QA:376:G:H5''   | 16:QP:5:ARG:HD3    | 1.92                     | 0.50              |
| 25:RA:839:U:H2'   | 25:RA:840:C:C6     | 2.46                     | 0.50              |
| 32:YI:78:THR:CA   | 32:YI:142:VAL:HG23 | 2.38                     | 0.50              |
| 13:XM:10:PRO:CG   | 13:XM:18:ALA:CA    | 2.86                     | 0.50              |
| 45:RZ:155:LEU:C   | 45:RZ:156:LYS:CG   | 2.68                     | 0.50              |
| 27:YD:43:ARG:HH11 | 27:YD:44:ASN:ND2   | 2.09                     | 0.50              |
| 25:RA:2439:A:C8   | 25:RA:2439:A:H5'   | 2.47                     | 0.50              |
| 21:XU:9:ARG:HH21  | 21:XU:10:ARG:HE    | 1.59                     | 0.50              |
| 1:QA:748:C:H4'    | 1:QA:749:C:O5'     | 2.11                     | 0.50              |
| 43:YX:36:LYS:HG3  | 43:YX:54:VAL:HB    | 1.92                     | 0.50              |
| 26:RB:79:C:C2'    | 26:RB:80:U:H5'     | 2.41                     | 0.50              |
| 25:RA:2262:U:H2'  | 25:RA:2263:C:H6    | 1.75                     | 0.50              |
| 1:XA:1411:C:H2'   | 1:XA:1412:C:H6     | 1.76                     | 0.50              |
| 1:XA:1148:U:H2'   | 1:XA:1149:C:O4'    | 2.11                     | 0.50              |
| 25:YA:1805:U:O2   | 27:YD:50:THR:HB    | 2.11                     | 0.50              |
| 36:RQ:34:LEU:HB2  | 36:RQ:118:LEU:HD22 | 1.92                     | 0.50              |
| 26:YB:6:C:HO2'    | 38:YS:29:PHE:HE1   | 1.57                     | 0.50              |
| 25:YA:579:G:O2'   | 25:YA:2019:A:OP1   | 2.26                     | 0.50              |
| 25:RA:388:G:H5'   | 47:R1:25:LYS:HB2   | 1.92                     | 0.50              |
| 31:RH:10:PRO:C    | 31:RH:11:VAL:CG1   | 2.79                     | 0.50              |
| 13:XM:10:PRO:HG2  | 13:XM:18:ALA:CA    | 2.40                     | 0.50              |
| 24:QY:55:PRO:HD3  | 24:QY:64:TRP:CZ3   | 2.47                     | 0.50              |
| 25:RA:593:G:O4'   | 54:R8:4:MET:HE1    | 2.12                     | 0.50              |
| 9:XI:27:THR:HG21  | 9:XI:32:ASP:HA     | 1.94                     | 0.50              |
| 10:XJ:79:ARG:HD3  | 10:XJ:79:ARG:H     | 1.76                     | 0.50              |
| 25:YA:2404:C:O3'  | 35:YP:77:ARG:NH2   | 2.45                     | 0.50              |
| 44:RY:48:ALA:O    | 44:RY:50:ARG:N     | 2.44                     | 0.50              |
| 2:XB:48:MET:HA    | 2:XB:51:LEU:HD12   | 1.94                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:QI:82:ALA:HB1   | 9:QI:96:LEU:HD21   | 1.93                     | 0.50              |
| 2:QB:18:GLY:HA2   | 2:QB:40:HIS:O      | 2.11                     | 0.50              |
| 39:RT:107:ASP:OD1 | 39:RT:107:ASP:N    | 2.43                     | 0.50              |
| 25:YA:817:C:H4'   | 25:YA:932:G:C5     | 2.46                     | 0.50              |
| 25:RA:859:G:HO2'  | 25:RA:860:U:H6     | 1.57                     | 0.50              |
| 2:XB:132:LYS:O    | 2:XB:134:GLU:N     | 2.44                     | 0.50              |
| 40:RU:74:LEU:HD13 | 40:RU:79:PHE:HB2   | 1.92                     | 0.50              |
| 25:RA:2313:C:H4'  | 30:RG:91:ARG:HG3   | 1.92                     | 0.50              |
| 25:YA:1858:G:H1'  | 25:YA:1884:A:H61   | 1.76                     | 0.50              |
| 41:YV:62:LEU:HB3  | 41:YV:93:GLU:O     | 2.12                     | 0.50              |
| 11:QK:20:TYR:CE2  | 11:QK:83:ILE:HD12  | 2.46                     | 0.50              |
| 25:RA:1625:C:H2'  | 25:RA:1626:G:O4'   | 2.10                     | 0.50              |
| 1:QA:1286:A:H8    | 1:QA:1287:A:H4'    | 1.76                     | 0.50              |
| 25:RA:296:C:H2'   | 25:RA:297:C:C6     | 2.47                     | 0.50              |
| 13:XM:8:GLU:O     | 13:XM:8:GLU:HG3    | 2.10                     | 0.50              |
| 1:QA:960:U:H4'    | 1:QA:961:U:OP2     | 2.12                     | 0.50              |
| 1:QA:674:G:H2'    | 1:QA:675:A:H8      | 1.75                     | 0.50              |
| 9:XI:28:VAL:HG22  | 9:XI:29:ASN:N      | 2.26                     | 0.50              |
| 25:RA:764:A:H5''  | 27:RD:210:GLY:HA2  | 1.93                     | 0.50              |
| 1:QA:954:G:H21    | 1:QA:1227:A:H62    | 1.59                     | 0.50              |
| 30:YG:36:LYS:HD2  | 30:YG:160:VAL:HG21 | 1.93                     | 0.50              |
| 3:XC:23:TYR:HD2   | 10:XJ:10:GLY:HA2   | 1.76                     | 0.50              |
| 1:XA:1293:G:H2'   | 1:XA:1294:G:H8     | 1.75                     | 0.50              |
| 1:QA:1286:A:C8    | 1:QA:1287:A:H4'    | 2.47                     | 0.50              |
| 46:R0:37:LEU:N    | 46:R0:59:LEU:O     | 2.32                     | 0.50              |
| 25:RA:2233:U:H2'  | 25:RA:2234:G:C8    | 2.46                     | 0.50              |
| 45:YZ:74:VAL:HG13 | 45:YZ:86:VAL:HG22  | 1.94                     | 0.50              |
| 25:RA:1070:A:H5'  | 25:RA:1071:G:H5''  | 1.91                     | 0.50              |
| 30:RG:107:LEU:HA  | 30:RG:111:LEU:HD12 | 1.93                     | 0.50              |
| 31:RH:7:LEU:HD12  | 31:RH:65:HIS:CE1   | 2.47                     | 0.50              |
| 13:XM:9:ILE:HG12  | 13:XM:10:PRO:N     | 2.26                     | 0.50              |
| 52:Y6:8:LYS:HA    | 52:Y6:27:LYS:HA    | 1.93                     | 0.50              |
| 25:RA:614:U:O5'   | 25:RA:614:U:O2     | 2.30                     | 0.50              |
| 23:XX:5:A:H2'     | 23:XX:6:G:C8       | 2.42                     | 0.50              |
| 44:RY:73:ARG:HH21 | 44:RY:82:PRO:HD3   | 1.77                     | 0.50              |
| 19:QS:45:VAL:HG13 | 19:QS:62:ILE:HG22  | 1.94                     | 0.50              |
| 28:RE:29:GLY:O    | 28:RE:51:PHE:HE2   | 1.95                     | 0.50              |
| 4:XD:127:THR:HG23 | 4:XD:147:ALA:HB3   | 1.92                     | 0.50              |
| 4:QD:195:ALA:HB3  | 6:XF:16:GLN:O      | 2.11                     | 0.50              |
| 25:YA:2148:G:H2'  | 25:YA:2149:G:C8    | 2.47                     | 0.50              |
| 10:XJ:9:ARG:HB2   | 10:XJ:95:GLU:HB3   | 1.92                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:XA:512:U:H2'     | 1:XA:513:C:C6       | 2.47                     | 0.50              |
| 25:RA:271(A):A:H5' | 25:RA:271(B):C:OP2  | 2.10                     | 0.50              |
| 33:YN:12:ARG:O     | 33:YN:50:ASP:HB2    | 2.11                     | 0.50              |
| 11:XK:20:TYR:CE2   | 11:XK:83:ILE:HD12   | 2.47                     | 0.50              |
| 20:QT:89:ARG:HB2   | 20:QT:104:LEU:HD21  | 1.94                     | 0.50              |
| 25:RA:1759:A:C8    | 25:RA:2696:U:H1'    | 2.46                     | 0.50              |
| 35:YP:63:PRO:HB3   | 54:Y8:13:ARG:HG2    | 1.94                     | 0.50              |
| 44:YY:77:PRO:O     | 44:YY:78:ALA:HB2    | 2.12                     | 0.50              |
| 35:YP:52:GLU:HG2   | 35:YP:55:ARG:HH11   | 1.77                     | 0.50              |
| 25:YA:2712:U:O2'   | 25:YA:2712(A):A:O5' | 2.30                     | 0.50              |
| 25:RA:2130:U:O2    | 25:RA:2133:G:O2'    | 2.30                     | 0.50              |
| 1:XA:315:A:O2'     | 1:XA:316:G:OP2      | 2.29                     | 0.50              |
| 41:RV:5:VAL:HB     | 41:RV:37:VAL:HG21   | 1.93                     | 0.50              |
| 28:YE:116:VAL:O    | 28:YE:117:MET:HB3   | 2.12                     | 0.50              |
| 1:XA:745:C:OP1     | 1:XA:851:G:O2'      | 2.29                     | 0.50              |
| 5:XE:82:VAL:HG21   | 5:XE:138:ALA:HA     | 1.93                     | 0.50              |
| 25:RA:2245:U:H5'   | 25:RA:2246:G:H5'    | 1.94                     | 0.50              |
| 10:QJ:53:PRO:HA    | 14:QN:42:ILE:HD12   | 1.93                     | 0.50              |
| 13:XM:73:GLU:O     | 13:XM:77:ASN:N      | 2.43                     | 0.50              |
| 19:QS:21:GLU:HG3   | 19:QS:22:LEU:HD22   | 1.93                     | 0.50              |
| 52:Y6:23:THR:OG1   | 54:Y8:34:TRP:O      | 2.29                     | 0.50              |
| 11:XK:10:VAL:HG12  | 11:XK:11:LYS:HG2    | 1.94                     | 0.50              |
| 25:RA:1963:U:C2'   | 25:RA:1963:U:O2     | 2.60                     | 0.50              |
| 25:YA:363(E):U:H3' | 25:YA:363(F):A:C8   | 2.46                     | 0.50              |
| 18:XR:40:LEU:HB3   | 18:XR:79:LEU:HD11   | 1.93                     | 0.50              |
| 31:RH:10:PRO:O     | 31:RH:11:VAL:O      | 2.30                     | 0.50              |
| 25:RA:2393:A:H62   | 25:RA:2422:A:H61    | 1.58                     | 0.50              |
| 25:RA:2712:U:O2'   | 25:RA:2712(A):A:O5' | 2.30                     | 0.50              |
| 1:QA:328:C:C4'     | 1:QA:329:A:O5'      | 2.58                     | 0.50              |
| 33:YN:26:LEU:O     | 33:YN:30:ILE:HG13   | 2.11                     | 0.50              |
| 35:YP:138:LEU:HD11 | 35:YP:144:GLU:HG2   | 1.93                     | 0.50              |
| 1:QA:518:C:H2'     | 1:QA:530:G:H8       | 1.77                     | 0.50              |
| 30:RG:47:LYS:HG3   | 30:RG:82:LEU:HG     | 1.93                     | 0.50              |
| 25:RA:2529:G:OP2   | 25:RA:2530:A:H8     | 1.94                     | 0.50              |
| 4:XD:162:LEU:HD13  | 4:XD:181:MET:HG2    | 1.92                     | 0.50              |
| 27:YD:267:SER:C    | 27:YD:269:PHE:H     | 2.15                     | 0.50              |
| 27:YD:267:SER:O    | 27:YD:269:PHE:N     | 2.45                     | 0.50              |
| 1:QA:37:U:O2'      | 1:QA:500:G:H4'      | 2.11                     | 0.50              |
| 25:RA:1863:G:HO2'  | 25:RA:2411:A:HO2'   | 1.55                     | 0.50              |
| 26:YB:89:G:C6      | 26:YB:89(A):A:C6    | 3.00                     | 0.50              |
| 2:XB:17:PHE:HA     | 2:XB:204:ASN:OD1    | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RA:1281:G:H5'  | 25:RA:1282:U:OP2  | 2.11                     | 0.50              |
| 33:RN:73:THR:HB   | 33:RN:82:LEU:HD11 | 1.94                     | 0.50              |
| 44:RY:95:LYS:NZ   | 44:RY:99:CYS:O    | 2.42                     | 0.50              |
| 13:XM:9:ILE:HG12  | 13:XM:10:PRO:HD2  | 1.91                     | 0.50              |
| 35:YP:11:GLY:O    | 35:YP:13:ASN:N    | 2.42                     | 0.50              |
| 40:YU:92:ARG:HH22 | 41:YV:10:LYS:CA   | 2.25                     | 0.50              |
| 31:RH:54:ARG:HD3  | 31:RH:54:ARG:H    | 1.77                     | 0.50              |
| 39:RT:20:PRO:HD2  | 39:RT:86:ILE:HG23 | 1.94                     | 0.50              |
| 25:RA:2867:G:O2'  | 25:RA:2868:A:H8   | 1.94                     | 0.50              |
| 19:XS:40:ILE:HG12 | 19:XS:69:HIS:O    | 2.12                     | 0.50              |
| 1:QA:354:G:N2     | 1:QA:355:C:C2     | 2.79                     | 0.50              |
| 43:RX:63:LYS:H    | 43:RX:63:LYS:NZ   | 2.10                     | 0.50              |
| 25:YA:2467:C:H4'  | 36:YQ:123:HIS:CE1 | 2.47                     | 0.50              |
| 1:QA:1316:G:H4'   | 14:QN:18:VAL:HG11 | 1.93                     | 0.50              |
| 25:YA:2472:G:N1   | 25:YA:2477:C:OP1  | 2.30                     | 0.50              |
| 30:RG:43:LEU:HD22 | 30:RG:90:LEU:HD23 | 1.94                     | 0.50              |
| 11:XK:48:ILE:HD11 | 11:XK:64:ALA:HA   | 1.94                     | 0.50              |
| 25:RA:94(A):G:H2' | 25:RA:95:G:O4'    | 2.12                     | 0.50              |
| 1:XA:142:G:H2'    | 1:XA:143:A:H8     | 1.77                     | 0.50              |
| 22:QW:65:C:H2'    | 22:QW:66:C:C6     | 2.47                     | 0.50              |
| 1:QA:1072:G:H2'   | 1:QA:1073:U:C6    | 2.47                     | 0.50              |
| 47:Y1:7:ILE:HD13  | 47:Y1:69:LYS:HB3  | 1.92                     | 0.50              |
| 1:XA:337:C:H2'    | 1:XA:338:A:H8     | 1.77                     | 0.50              |
| 40:YU:113:ALA:O   | 40:YU:117:GLN:HB2 | 2.12                     | 0.50              |
| 25:RA:519:U:H2'   | 25:RA:520:G:H8    | 1.76                     | 0.50              |
| 25:YA:1336:A:P    | 43:YX:64:LYS:HZ2  | 2.35                     | 0.50              |
| 54:R8:34:TRP:O    | 54:R8:36:LYS:HG3  | 2.12                     | 0.50              |
| 45:RZ:45:ASP:O    | 45:RZ:49:ARG:HG2  | 2.12                     | 0.50              |
| 25:YA:1264:G:H3'  | 25:YA:1265:A:H5'' | 1.93                     | 0.50              |
| 1:XA:1260:C:O5'   | 1:XA:1284:C:H4'   | 2.12                     | 0.50              |
| 25:YA:2115:G:O2'  | 25:YA:2171:A:N6   | 2.44                     | 0.50              |
| 54:R8:6:THR:HG21  | 54:R8:63:PRO:HD3  | 1.94                     | 0.50              |
| 41:RV:48:GLY:O    | 41:RV:49:THR:O    | 2.30                     | 0.50              |
| 35:YP:60:MET:C    | 35:YP:61:ARG:HG2  | 2.32                     | 0.50              |
| 19:QS:40:ILE:HG21 | 19:QS:66:MET:O    | 2.12                     | 0.50              |
| 25:YA:263:C:H2'   | 25:YA:264:C:O4'   | 2.12                     | 0.50              |
| 25:RA:1285:G:N2   | 25:RA:1328:G:H5'' | 2.27                     | 0.50              |
| 27:YD:109:ASP:N   | 27:YD:196:VAL:O   | 2.44                     | 0.50              |
| 25:YA:78:A:H2'    | 25:YA:79:G:H8     | 1.75                     | 0.50              |
| 1:QA:530:G:N3     | 23:QX:21:A2M:H2   | 2.27                     | 0.50              |
| 1:XA:35:G:H2'     | 1:XA:36:C:C6      | 2.47                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:XJ:38:ILE:HB    | 10:XJ:71:LEU:HB3   | 1.94                     | 0.50              |
| 1:QA:1065:U:OP2    | 1:QA:1190:G:N2     | 2.41                     | 0.50              |
| 1:QA:534:U:H5'     | 1:QA:535:A:OP2     | 2.12                     | 0.50              |
| 25:RA:1165:U:H2'   | 25:RA:1166:C:C6    | 2.47                     | 0.50              |
| 25:RA:2345:G:N3    | 25:RA:2381:C:H2'   | 2.26                     | 0.50              |
| 28:YE:120:TRP:CD1  | 28:YE:155:LYS:HB3  | 2.47                     | 0.50              |
| 44:YY:52:SER:HA    | 44:YY:56:PRO:HA    | 1.94                     | 0.50              |
| 7:XG:76:ARG:HD2    | 7:XG:89:MET:HG3    | 1.94                     | 0.50              |
| 29:YF:83:PHE:O     | 29:YF:85:GLY:N     | 2.45                     | 0.50              |
| 25:RA:2445:G:C2'   | 25:RA:2446:G:H5'   | 2.42                     | 0.49              |
| 1:QA:1490:C:O2'    | 1:QA:1491:G:H5''   | 2.12                     | 0.49              |
| 25:RA:2091:U:H1'   | 47:R1:47:GLN:NE2   | 2.27                     | 0.49              |
| 1:QA:1330:U:H3'    | 1:QA:1331:G:O4'    | 2.12                     | 0.49              |
| 1:QA:1226:C:H4'    | 19:QS:80:TYR:CZ    | 2.47                     | 0.49              |
| 46:Y0:3:HIS:ND1    | 46:Y0:3:HIS:O      | 2.43                     | 0.49              |
| 34:RO:104:ARG:HG2  | 34:RO:121:VAL:HG12 | 1.94                     | 0.49              |
| 31:RH:153:LYS:HB3  | 31:RH:161:GLY:HA2  | 1.94                     | 0.49              |
| 31:RH:147:ASN:O    | 31:RH:151:ILE:HG12 | 2.12                     | 0.49              |
| 25:YA:363(F):A:H1' | 25:YA:364:C:H5     | 1.75                     | 0.49              |
| 1:XA:1490:C:O2'    | 1:XA:1491:G:H5'    | 2.12                     | 0.49              |
| 10:QJ:48:THR:HA    | 10:QJ:62:HIS:HB3   | 1.93                     | 0.49              |
| 26:RB:89(A):A:N7   | 26:RB:90:C:H1'     | 2.27                     | 0.49              |
| 25:YA:2046:G:H5'   | 51:Y5:19:ARG:HG3   | 1.93                     | 0.49              |
| 4:QD:166:LYS:HD2   | 27:YD:134:ARG:NH1  | 2.26                     | 0.49              |
| 45:YZ:126:VAL:HG12 | 45:YZ:163:LEU:HA   | 1.94                     | 0.49              |
| 2:XB:146:GLN:O     | 2:XB:150:SER:HB3   | 2.12                     | 0.49              |
| 22:QV:9:G:O2'      | 22:QV:10:G:N7      | 2.41                     | 0.49              |
| 25:YA:2855:C:H2'   | 25:YA:2856:C:C6    | 2.47                     | 0.49              |
| 2:QB:103:THR:HA    | 2:QB:180:LEU:HD11  | 1.93                     | 0.49              |
| 1:XA:1101:A:H4'    | 1:XA:1102:A:O5'    | 2.12                     | 0.49              |
| 25:RA:2446:G:C3'   | 25:RA:2447:G:C5'   | 2.90                     | 0.49              |
| 54:Y8:6:THR:OG1    | 54:Y8:6:THR:O      | 2.26                     | 0.49              |
| 40:RU:92:ARG:HG3   | 40:RU:95:LEU:H     | 1.76                     | 0.49              |
| 38:YS:71:ARG:HH12  | 38:YS:106:ARG:HH21 | 1.60                     | 0.49              |
| 5:QE:12:LEU:HD12   | 5:QE:128:PRO:CB    | 2.41                     | 0.49              |
| 4:XD:111:ALA:HB2   | 4:XD:120:LEU:HD12  | 1.94                     | 0.49              |
| 25:RA:2199:A:C5    | 25:RA:2225:A:C5    | 3.01                     | 0.49              |
| 25:RA:1113:U:H2'   | 25:RA:1114:G:C8    | 2.47                     | 0.49              |
| 25:YA:1907:G:C2'   | 25:YA:1908:C:H5'   | 2.42                     | 0.49              |
| 1:XA:7:G:H2'       | 5:XE:119:LEU:HD22  | 1.93                     | 0.49              |
| 1:XA:1512:U:H2'    | 1:XA:1513:A:H8     | 1.76                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:XG:20:ASP:OD1    | 7:XG:23:VAL:HB     | 2.12                     | 0.49              |
| 45:YZ:124:ILE:HD11 | 45:YZ:165:VAL:HG11 | 1.94                     | 0.49              |
| 25:YA:1384:A:N3    | 25:YA:1405:U:H1'   | 2.28                     | 0.49              |
| 45:RZ:165:VAL:HG13 | 45:RZ:166:SER:H    | 1.76                     | 0.49              |
| 25:RA:2876:G:O2'   | 39:RT:3:ARG:NH1    | 2.45                     | 0.49              |
| 1:XA:1456:G:N1     | 20:XT:55:ILE:HD11  | 2.27                     | 0.49              |
| 1:XA:1273:G:H3'    | 1:XA:1274:G:H8     | 1.76                     | 0.49              |
| 1:XA:222:U:H2'     | 1:XA:223:U:C6      | 2.47                     | 0.49              |
| 41:RV:2:PHE:CD2    | 41:RV:42:GLY:HA2   | 2.46                     | 0.49              |
| 2:XB:82:ARG:O      | 2:XB:86:GLU:HG2    | 2.12                     | 0.49              |
| 1:QA:652:U:O4      | 1:QA:752:G:O2'     | 2.25                     | 0.49              |
| 7:QG:113:GLU:HB2   | 7:QG:119:ARG:HG2   | 1.94                     | 0.49              |
| 6:XF:83:ASP:OD2    | 6:XF:83:ASP:N      | 2.45                     | 0.49              |
| 25:YA:2776:A:OP1   | 25:YA:2776:A:H3'   | 2.12                     | 0.49              |
| 1:XA:41:G:H2'      | 1:XA:42:G:C8       | 2.48                     | 0.49              |
| 25:YA:2191:G:O2'   | 25:YA:2192:G:OP1   | 2.26                     | 0.49              |
| 44:YY:62:GLU:CD    | 44:YY:63:LYS:H     | 2.15                     | 0.49              |
| 25:YA:270(I):G:H1  | 25:YA:270(Q):C:H42 | 1.60                     | 0.49              |
| 25:YA:2748:A:H2    | 25:YA:2754:U:H3    | 1.58                     | 0.49              |
| 25:YA:2527:C:H5'   | 55:Y9:30:PRO:HB2   | 1.92                     | 0.49              |
| 1:QA:1213:A:N6     | 1:QA:1215:G:N3     | 2.60                     | 0.49              |
| 27:YD:65:ILE:HD11  | 27:YD:67:PHE:CZ    | 2.47                     | 0.49              |
| 52:R6:15:GLU:OE1   | 52:R6:18:ARG:HB2   | 2.12                     | 0.49              |
| 23:XX:20:A2M:HM'2  | 24:XY:91:TYR:HB2   | 1.94                     | 0.49              |
| 25:YA:918:A:N3     | 26:YB:80:U:O2'     | 2.44                     | 0.49              |
| 31:RH:6:ARG:HB3    | 31:RH:54:ARG:HH12  | 1.77                     | 0.49              |
| 25:RA:2207:G:H3'   | 25:RA:2208:A:N3    | 2.26                     | 0.49              |
| 19:QS:42:PRO:CG    | 50:R4:60:GLN:HG3   | 2.42                     | 0.49              |
| 1:QA:1137:C:H4'    | 1:QA:1138:G:O5'    | 2.11                     | 0.49              |
| 25:YA:2562:U:H1'   | 34:YO:23:ARG:HH11  | 1.77                     | 0.49              |
| 25:YA:2442:C:H2'   | 25:YA:2443:C:H6    | 1.77                     | 0.49              |
| 5:QE:87:SER:HB3    | 5:QE:131:ILE:HD13  | 1.94                     | 0.49              |
| 5:QE:79:GLU:HG3    | 5:QE:93:PRO:HD2    | 1.94                     | 0.49              |
| 52:Y6:7:ILE:H      | 52:Y6:7:ILE:HD13   | 1.77                     | 0.49              |
| 1:QA:766:A:H2'     | 1:QA:767:A:O4'     | 2.11                     | 0.49              |
| 25:YA:928:G:H3'    | 25:YA:929:G:C8     | 2.47                     | 0.49              |
| 44:RY:76:CYS:O     | 44:RY:77:PRO:C     | 2.50                     | 0.49              |
| 25:YA:6:A:N3       | 25:YA:7:G:C8       | 2.80                     | 0.49              |
| 27:YD:43:ARG:HB3   | 27:YD:54:ARG:HB2   | 1.94                     | 0.49              |
| 52:Y6:6:ARG:HG2    | 52:Y6:8:LYS:N      | 2.24                     | 0.49              |
| 25:RA:1917:U:C2'   | 25:RA:1918:A:H5'   | 2.42                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:XB:24:TRP:CD1    | 2:XB:24:TRP:N      | 2.80                     | 0.49              |
| 31:RH:94:TYR:CD2   | 31:RH:107:VAL:HG12 | 2.47                     | 0.49              |
| 1:QA:707:C:H2'     | 1:QA:708:C:H6      | 1.78                     | 0.49              |
| 25:RA:2529:G:H22   | 55:R9:31:LYS:NZ    | 2.09                     | 0.49              |
| 25:RA:2059:A:H5'   | 25:RA:2060:A:OP2   | 2.12                     | 0.49              |
| 1:QA:222:U:H2'     | 1:QA:223:U:C6      | 2.47                     | 0.49              |
| 3:QC:116:VAL:HG21  | 3:QC:202:ILE:HD11  | 1.93                     | 0.49              |
| 1:QA:793:U:H5'     | 1:QA:794:A:O5'     | 2.13                     | 0.49              |
| 45:YZ:91:LEU:HD12  | 45:YZ:130:PRO:HB3  | 1.95                     | 0.49              |
| 41:RV:76:LYS:HB3   | 41:RV:79:VAL:HG23  | 1.94                     | 0.49              |
| 15:XO:39:LEU:HD12  | 15:XO:56:LEU:HB2   | 1.94                     | 0.49              |
| 30:RG:114:ILE:HD11 | 30:RG:140:ILE:HD13 | 1.94                     | 0.49              |
| 30:RG:135:LEU:HD23 | 30:RG:140:ILE:HD11 | 1.93                     | 0.49              |
| 1:QA:555:C:H2'     | 1:QA:556:C:C6      | 2.47                     | 0.49              |
| 25:YA:2750:A:H2'   | 25:YA:2752:C:N4    | 2.27                     | 0.49              |
| 25:YA:2844:G:H3'   | 25:YA:2845:G:H8    | 1.77                     | 0.49              |
| 25:YA:278:A:H61    | 25:YA:362:U:H3     | 1.59                     | 0.49              |
| 31:YH:105:LEU:HD12 | 31:YH:113:VAL:HB   | 1.95                     | 0.49              |
| 28:RE:35:GLN:HG3   | 28:RE:64:LYS:HZ2   | 1.77                     | 0.49              |
| 44:YY:20:TYR:CZ    | 44:YY:42:VAL:HA    | 2.47                     | 0.49              |
| 4:XD:7:PRO:HB2     | 4:XD:10:ARG:HD2    | 1.94                     | 0.49              |
| 4:QD:79:PHE:HE1    | 4:QD:204:ILE:HD13  | 1.76                     | 0.49              |
| 19:XS:40:ILE:HG21  | 19:XS:66:MET:O     | 2.12                     | 0.49              |
| 25:YA:2232:U:P     | 47:Y1:40:ARG:HH12  | 2.34                     | 0.49              |
| 37:RR:37:THR:HG22  | 37:RR:39:PRO:HD2   | 1.95                     | 0.49              |
| 15:QO:16:ALA:HB1   | 15:QO:21:ASP:HB3   | 1.94                     | 0.49              |
| 44:YY:87:LYS:HB3   | 44:YY:92:ASN:HB3   | 1.95                     | 0.49              |
| 30:YG:145:THR:O    | 30:YG:147:ASP:N    | 2.43                     | 0.49              |
| 1:XA:878:G:H5'     | 8:XH:89:PRO:HG2    | 1.94                     | 0.49              |
| 6:QF:42:GLU:OE2    | 6:QF:59:TYR:OH     | 2.29                     | 0.49              |
| 53:R7:24:THR:HG23  | 53:R7:27:GLY:HA3   | 1.95                     | 0.49              |
| 25:RA:620:G:N3     | 25:RA:620:G:H5'    | 2.27                     | 0.49              |
| 1:QA:1517:G:H1'    | 25:RA:1919:A:O3'   | 2.13                     | 0.49              |
| 1:QA:1109:C:OP2    | 3:QC:176:HIS:ND1   | 2.41                     | 0.49              |
| 38:RS:24:LEU:HB2   | 38:RS:85:VAL:HG12  | 1.93                     | 0.49              |
| 31:YH:107:VAL:HG23 | 31:YH:108:GLY:H    | 1.76                     | 0.49              |
| 25:YA:1281:G:H5'   | 25:YA:1282:U:OP2   | 2.12                     | 0.49              |
| 2:QB:112:VAL:HG22  | 2:QB:149:LEU:HD13  | 1.95                     | 0.49              |
| 14:XN:41:ARG:NE    | 14:XN:42:ILE:CD1   | 2.76                     | 0.49              |
| 35:YP:64:LYS:HB3   | 54:Y8:25:MET:HG2   | 1.94                     | 0.49              |
| 25:RA:69:C:O2      | 25:RA:69:C:O4'     | 2.29                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:Y4:55:ARG:HH21 | 50:Y4:56:VAL:HG12 | 1.77                     | 0.49              |
| 31:YH:54:ARG:NE   | 31:YH:57:ASP:OD1  | 2.42                     | 0.49              |
| 39:RT:16:ARG:NH2  | 39:RT:19:LEU:HD21 | 2.28                     | 0.49              |
| 1:XA:1152:A:H2'   | 1:XA:1153:C:C6    | 2.46                     | 0.49              |
| 3:QC:108:ASN:ND2  | 3:QC:144:SER:HB2  | 2.27                     | 0.49              |
| 39:RT:26:ASP:CB   | 39:RT:91:ARG:HA   | 2.42                     | 0.49              |
| 1:QA:611:A:H61    | 1:QA:629:G:H1     | 1.59                     | 0.49              |
| 45:RZ:110:GLY:O   | 45:RZ:112:ARG:N   | 2.44                     | 0.49              |
| 25:RA:1814:G:H4'  | 27:RD:51:VAL:HG21 | 1.93                     | 0.49              |
| 30:YG:9:ARG:O     | 30:YG:13:GLU:HG2  | 2.12                     | 0.49              |
| 28:YE:128:SER:OG  | 28:YE:129:HIS:N   | 2.44                     | 0.49              |
| 25:YA:1266:G:O5'  | 42:YW:15:ARG:NH2  | 2.45                     | 0.49              |
| 45:RZ:58:VAL:O    | 45:RZ:59:LEU:CB   | 2.61                     | 0.49              |
| 25:RA:1224:C:H5'' | 41:RV:85:LYS:HE2  | 1.94                     | 0.49              |
| 25:YA:833:U:H5''  | 35:YP:48:PRO:HB2  | 1.94                     | 0.49              |
| 1:XA:1305:G:N2    | 1:XA:1331:G:H2'   | 2.22                     | 0.49              |
| 29:YF:24:LEU:HD13 | 29:YF:25:PRO:HD2  | 1.93                     | 0.49              |
| 1:QA:523:A:H61    | 12:QL:53:ARG:NH1  | 2.09                     | 0.49              |
| 25:RA:1019:U:O2'  | 25:RA:1021:A:H2   | 1.95                     | 0.49              |
| 10:XJ:40:LEU:HG   | 10:XJ:41:PRO:HD2  | 1.94                     | 0.49              |
| 37:YR:42:LYS:HA   | 37:YR:45:ARG:HE   | 1.77                     | 0.49              |
| 1:QA:1070:U:OP1   | 5:QE:18:ARG:NH1   | 2.46                     | 0.49              |
| 52:R6:12:GLU:HA   | 52:R6:24:GLU:HB3  | 1.94                     | 0.49              |
| 54:R8:34:TRP:C    | 54:R8:36:LYS:H    | 2.16                     | 0.49              |
| 11:XK:13:GLN:NE2  | 11:XK:76:GLY:HA3  | 2.28                     | 0.49              |
| 9:QI:19:LEU:HB3   | 9:QI:59:PHE:HB3   | 1.94                     | 0.49              |
| 1:QA:1541:U:O2'   | 18:QR:18:ARG:NH2  | 2.44                     | 0.49              |
| 25:YA:2563:U:H4'  | 34:YO:28:SER:HA   | 1.95                     | 0.49              |
| 28:RE:70:ALA:O    | 28:RE:72:VAL:N    | 2.46                     | 0.49              |
| 11:QK:21:ILE:HG12 | 11:QK:30:VAL:HG12 | 1.94                     | 0.49              |
| 1:XA:706:A:O4'    | 11:XK:29:ILE:HD11 | 2.13                     | 0.49              |
| 32:YI:8:PRO:HD3   | 32:YI:15:VAL:HG22 | 1.95                     | 0.49              |
| 22:QW:34:C:H42    | 23:QX:14:A:N6     | 2.11                     | 0.49              |
| 22:QW:32:C:C5     | 22:QW:33:U:C4     | 3.01                     | 0.49              |
| 1:XA:960:U:C2'    | 1:XA:961:U:OP2    | 2.61                     | 0.49              |
| 34:RO:98:VAL:CG1  | 34:RO:117:LEU:HB3 | 2.43                     | 0.49              |
| 25:RA:2091:U:H5'' | 25:RA:2092:U:C5'  | 2.43                     | 0.49              |
| 1:QA:579:G:H5'    | 1:QA:728:A:H1'    | 1.94                     | 0.49              |
| 1:QA:1380:U:H5    | 7:QG:3:ARG:HG2    | 1.76                     | 0.49              |
| 1:XA:708:C:H2'    | 1:XA:709:G:H8     | 1.78                     | 0.49              |
| 40:RU:81:HIS:CD2  | 40:RU:84:LYS:HD3  | 2.48                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:RG:120:LEU:N    | 30:RG:179:PRO:O    | 2.43                     | 0.49              |
| 1:XA:337:C:H2'     | 1:XA:338:A:C8      | 2.47                     | 0.49              |
| 4:QD:163:GLU:OE1   | 4:QD:166:LYS:NZ    | 2.45                     | 0.49              |
| 15:QO:24:SER:OG    | 15:QO:25:THR:N     | 2.46                     | 0.49              |
| 6:QF:42:GLU:HG2    | 6:QF:42:GLU:O      | 2.11                     | 0.49              |
| 25:YA:453:C:O2     | 25:YA:457:A:O2'    | 2.29                     | 0.49              |
| 30:YG:97:ASP:O     | 30:YG:101:ILE:HG23 | 2.13                     | 0.49              |
| 28:YE:36:ARG:HH21  | 28:YE:88:GLY:HA3   | 1.77                     | 0.49              |
| 30:YG:104:GLU:HG2  | 50:Y4:23:GLU:HG3   | 1.94                     | 0.49              |
| 34:YO:25:LEU:HB2   | 34:YO:38:VAL:HG23  | 1.93                     | 0.49              |
| 24:QY:41:THR:N     | 24:QY:45:GLU:OE1   | 2.41                     | 0.49              |
| 16:QP:52:ASP:OD2   | 16:QP:54:GLU:HG2   | 2.13                     | 0.49              |
| 25:YA:807:U:OP2    | 35:YP:41:ARG:NH1   | 2.46                     | 0.49              |
| 34:YO:71:ARG:NH1   | 39:YT:74:ARG:HH21  | 2.10                     | 0.49              |
| 32:RI:2:LYS:HD2    | 32:RI:20:ASP:HB3   | 1.94                     | 0.49              |
| 10:QJ:46:ARG:HG2   | 10:QJ:64:GLU:HB3   | 1.94                     | 0.49              |
| 25:RA:1904:G:H2'   | 25:RA:1905:C:O4'   | 2.13                     | 0.49              |
| 30:RG:60:LEU:HD21  | 30:RG:92:VAL:CG1   | 2.41                     | 0.49              |
| 43:RX:36:LYS:HG3   | 43:RX:54:VAL:HB    | 1.95                     | 0.49              |
| 10:QJ:79:ARG:CZ    | 9:XI:94:ALA:HB1    | 2.42                     | 0.49              |
| 1:XA:1330:U:H3'    | 1:XA:1331:G:O4'    | 2.13                     | 0.49              |
| 25:YA:389:G:N1     | 35:YP:71:VAL:HG12  | 2.28                     | 0.49              |
| 25:YA:2016:U:C1'   | 51:Y5:6:VAL:CG1    | 2.90                     | 0.49              |
| 18:QR:23:LYS:HD2   | 18:QR:58:LEU:HB3   | 1.93                     | 0.49              |
| 1:XA:1512:U:H2'    | 1:XA:1513:A:C8     | 2.48                     | 0.49              |
| 1:QA:1001(A):G:OP1 | 1:QA:1001(A):G:H4' | 2.13                     | 0.49              |
| 3:QC:148:GLY:HA3   | 3:QC:172:ARG:O     | 2.12                     | 0.49              |
| 54:R8:34:TRP:O     | 54:R8:36:LYS:N     | 2.42                     | 0.49              |
| 9:QI:19:LEU:HD23   | 9:QI:61:ALA:HA     | 1.94                     | 0.49              |
| 39:RT:106:SER:HA   | 39:RT:110:ILE:HG13 | 1.95                     | 0.49              |
| 25:RA:2166:G:O2'   | 25:RA:2167:U:OP1   | 2.26                     | 0.49              |
| 2:XB:129:GLU:HB3   | 2:XB:130:ARG:NH1   | 2.27                     | 0.49              |
| 1:XA:1515:C:H2'    | 1:XA:1516:G:H8     | 1.77                     | 0.49              |
| 10:XJ:8:LEU:HD22   | 10:XJ:20:ALA:HB2   | 1.94                     | 0.49              |
| 25:YA:2320:A:N3    | 25:YA:2320:A:H2'   | 2.28                     | 0.49              |
| 25:YA:528:A:O2'    | 25:YA:529:A:H5''   | 2.12                     | 0.49              |
| 25:RA:1923:U:H2'   | 25:RA:1924:C:C6    | 2.48                     | 0.49              |
| 25:YA:1999:C:H5''  | 25:YA:2723:C:O2'   | 2.12                     | 0.49              |
| 35:RP:57:THR:HG21  | 35:RP:60:MET:CB    | 2.42                     | 0.49              |
| 25:RA:1697:G:H2'   | 25:RA:1698:A:OP1   | 2.13                     | 0.49              |
| 25:YA:2306:C:H5    | 30:YG:45:GLU:OE1   | 1.96                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 47:R1:85:LEU:HA   | 47:R1:87:PRO:HD2   | 1.94                     | 0.49              |
| 25:YA:1171:G:H1   | 25:YA:1178:C:N4    | 2.10                     | 0.49              |
| 25:RA:722:A:H5'   | 25:RA:723:G:OP2    | 2.13                     | 0.49              |
| 39:YT:26:ASP:CB   | 39:YT:91:ARG:HA    | 2.43                     | 0.49              |
| 1:XA:50:A:N1      | 1:XA:360:A:O2'     | 2.39                     | 0.49              |
| 25:RA:588:U:H1'   | 29:RF:90:PHE:CG    | 2.48                     | 0.49              |
| 25:YA:2881:C:H5'' | 37:YR:117:VAL:HG21 | 1.95                     | 0.49              |
| 7:QG:13:GLN:O     | 7:QG:24:THR:HG21   | 2.13                     | 0.49              |
| 33:YN:36:GLY:H    | 33:YN:42:TRP:HZ3   | 1.60                     | 0.49              |
| 29:YF:33:LEU:HD13 | 29:YF:112:MET:HE2  | 1.95                     | 0.49              |
| 5:XE:72:GLN:O     | 5:XE:75:THR:HG22   | 2.12                     | 0.49              |
| 1:XA:401:C:O2'    | 1:XA:621:A:N3      | 2.38                     | 0.49              |
| 36:YQ:27:VAL:HG13 | 45:YZ:81:ARG:HH22  | 1.78                     | 0.49              |
| 27:YD:71:ASP:HB3  | 27:YD:103:ARG:HH22 | 1.78                     | 0.49              |
| 15:XO:10:LYS:HD2  | 15:XO:10:LYS:HA    | 1.69                     | 0.49              |
| 25:YA:227:A:H5''  | 35:YP:76:LYS:NZ    | 2.27                     | 0.49              |
| 36:YQ:63:LYS:H    | 45:YZ:178:GLU:HG2  | 1.78                     | 0.49              |
| 26:YB:114:G:H2'   | 26:YB:115:G:H8     | 1.78                     | 0.49              |
| 44:RY:97:ARG:NH2  | 44:RY:98:VAL:HB    | 2.19                     | 0.48              |
| 25:YA:1204:A:H61  | 25:YA:1240:U:H2'   | 1.78                     | 0.48              |
| 1:XA:960:U:O2'    | 1:XA:961:U:OP2     | 2.30                     | 0.48              |
| 22:QV:53:G:H2'    | 22:QV:54:U:H6      | 1.76                     | 0.48              |
| 22:QV:52:G:C2'    | 22:QV:53:G:H5'     | 2.42                     | 0.48              |
| 25:YA:259:G:N2    | 25:YA:621:A:H8     | 2.07                     | 0.48              |
| 25:RA:614:U:O2    | 25:RA:614:U:O4'    | 2.29                     | 0.48              |
| 25:YA:2406:U:C2   | 35:YP:72:PRO:HB2   | 2.48                     | 0.48              |
| 13:QM:2:ALA:O     | 13:QM:4:ILE:N      | 2.46                     | 0.48              |
| 25:YA:2356:C:H4'  | 46:Y0:20:ARG:HG3   | 1.94                     | 0.48              |
| 5:XE:11:ILE:HD11  | 5:XE:33:VAL:HG23   | 1.96                     | 0.48              |
| 25:YA:2870:C:H2'  | 25:YA:2871:C:O4'   | 2.12                     | 0.48              |
| 1:QA:1002:G:N2    | 1:QA:1039:C:O2     | 2.45                     | 0.48              |
| 11:XK:44:SER:O    | 11:XK:48:ILE:HG12  | 2.13                     | 0.48              |
| 1:XA:1095:U:H5''  | 1:XA:1109:C:O2     | 2.13                     | 0.48              |
| 25:RA:1550:C:OP1  | 25:RA:1720:U:O2'   | 2.31                     | 0.48              |
| 1:QA:134:A:H61    | 16:QP:25:ARG:NH1   | 2.11                     | 0.48              |
| 46:Y0:50:ASN:HB3  | 46:Y0:63:VAL:HG22  | 1.94                     | 0.48              |
| 3:QC:76:VAL:HG13  | 3:QC:84:ILE:HG13   | 1.94                     | 0.48              |
| 40:YU:100:VAL:O   | 40:YU:101:ARG:HG2  | 2.13                     | 0.48              |
| 43:YX:26:TYR:HB3  | 43:YX:92:LEU:HD12  | 1.94                     | 0.48              |
| 25:YA:1133:U:H2'  | 25:YA:1137:G:OP1   | 2.13                     | 0.48              |
| 25:YA:451:C:H4'   | 29:YF:52:LYS:NZ    | 2.28                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:YA:815:C:H2'    | 25:YA:816:C:C6      | 2.48                     | 0.48              |
| 26:RB:34:U:H5''    | 26:RB:35:U:OP1      | 2.13                     | 0.48              |
| 26:YB:34:U:H5''    | 26:YB:35:U:OP1      | 2.12                     | 0.48              |
| 37:RR:73:VAL:O     | 37:RR:76:VAL:HG12   | 2.13                     | 0.48              |
| 1:XA:1158:C:N4     | 1:XA:1160:G:C8      | 2.80                     | 0.48              |
| 25:RA:310:A:OP1    | 44:RY:18:GLY:HA2    | 2.13                     | 0.48              |
| 25:RA:2393:A:H4'   | 35:RP:62:LEU:N      | 2.27                     | 0.48              |
| 25:RA:1982:C:H2'   | 25:RA:1982:C:O2     | 2.11                     | 0.48              |
| 38:YS:74:ALA:HB1   | 38:YS:107:GLU:HB3   | 1.95                     | 0.48              |
| 27:YD:30:GLU:HG3   | 27:YD:63:ARG:CZ     | 2.42                     | 0.48              |
| 25:YA:620:G:H4'    | 25:YA:621:A:H5''    | 1.95                     | 0.48              |
| 1:QA:345:C:OP2     | 39:RT:39:ARG:NH2    | 2.46                     | 0.48              |
| 28:RE:176:ILE:HB   | 28:RE:181:LEU:HB2   | 1.94                     | 0.48              |
| 1:XA:410:G:H3'     | 4:XD:25:ARG:HH21    | 1.78                     | 0.48              |
| 27:YD:196:VAL:HG12 | 27:YD:197:GLY:H     | 1.78                     | 0.48              |
| 25:YA:2144:U:H4'   | 25:YA:2145:C:OP1    | 2.13                     | 0.48              |
| 1:XA:511:C:HO2'    | 1:XA:512:U:H6       | 1.59                     | 0.48              |
| 1:XA:111:G:O6      | 1:XA:330:C:N4       | 2.45                     | 0.48              |
| 25:YA:2336:A:H61   | 46:Y0:43:THR:HG22   | 1.78                     | 0.48              |
| 1:XA:129(A):G:C6   | 1:XA:189(E):U:H4'   | 2.48                     | 0.48              |
| 1:QA:1118:C:H1'    | 1:QA:1179:A:C4      | 2.48                     | 0.48              |
| 22:XV:3:C:H42      | 22:XV:70:G:H1       | 1.61                     | 0.48              |
| 4:XD:194:LEU:HB3   | 4:XD:196:LEU:HD12   | 1.95                     | 0.48              |
| 7:XG:28:ASN:OD1    | 7:XG:36:LYS:NZ      | 2.46                     | 0.48              |
| 1:QA:1368:G:H5''   | 9:QI:112:LYS:HB3    | 1.95                     | 0.48              |
| 44:YY:48:ALA:N     | 44:YY:59:GLY:O      | 2.46                     | 0.48              |
| 1:QA:877:C:H5''    | 8:QH:88:LYS:HD2     | 1.94                     | 0.48              |
| 1:QA:769:G:H4'     | 1:QA:1513:A:H4'     | 1.94                     | 0.48              |
| 47:Y1:58:ILE:HG23  | 47:Y1:87:PRO:HG3    | 1.95                     | 0.48              |
| 19:XS:67:VAL:HG13  | 19:XS:68:GLY:H      | 1.78                     | 0.48              |
| 22:QV:54:U:O5'     | 22:QV:54:U:H6       | 1.95                     | 0.48              |
| 28:YE:38:THR:HG22  | 28:YE:40:GLU:H      | 1.78                     | 0.48              |
| 25:YA:1929:G:H4'   | 25:YA:1930:G:OP1    | 2.13                     | 0.48              |
| 30:YG:166:ASP:OD1  | 30:YG:166:ASP:N     | 2.35                     | 0.48              |
| 39:YT:26:ASP:O     | 39:YT:49:VAL:HG12   | 2.13                     | 0.48              |
| 2:XB:207:ALA:O     | 2:XB:211:ILE:HG13   | 2.13                     | 0.48              |
| 15:XO:17:ARG:HD3   | 15:XO:26:GLU:HG3    | 1.94                     | 0.48              |
| 34:RO:97:ARG:HG3   | 34:RO:97:ARG:NH1    | 2.28                     | 0.48              |
| 1:QA:1001:A:H3'    | 1:QA:1001(A):G:H5'' | 1.95                     | 0.48              |
| 1:QA:277:C:H2'     | 1:QA:278:G:H8       | 1.78                     | 0.48              |
| 1:QA:1132:C:H2'    | 1:QA:1133:G:H8      | 1.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:RI:84:GLY:O    | 32:RI:86:THR:N    | 2.46                     | 0.48              |
| 55:Y9:9:ARG:NH1   | 55:Y9:14:CYS:O    | 2.47                     | 0.48              |
| 25:YA:1686:C:H2'  | 25:YA:1687:G:O4'  | 2.13                     | 0.48              |
| 1:QA:1521:G:H2'   | 1:QA:1522:U:H6    | 1.78                     | 0.48              |
| 1:XA:308:C:H2'    | 1:XA:309:G:H8     | 1.78                     | 0.48              |
| 28:RE:111:ARG:HA  | 37:RR:2:ARG:HH12  | 1.78                     | 0.48              |
| 33:RN:90:MET:HB3  | 33:RN:98:VAL:HG12 | 1.95                     | 0.48              |
| 25:RA:1914:C:OP1  | 25:RA:1914:C:O3'  | 2.31                     | 0.48              |
| 1:XA:1285:A:O2'   | 1:XA:1286:A:H5''  | 2.12                     | 0.48              |
| 27:RD:10:THR:HG23 | 27:RD:13:ARG:HB2  | 1.94                     | 0.48              |
| 10:XJ:54:PHE:CD1  | 10:XJ:55:LYS:HG3  | 2.48                     | 0.48              |
| 1:XA:579:G:H5'    | 1:XA:728:A:H1'    | 1.95                     | 0.48              |
| 31:RH:52:VAL:HG12 | 31:RH:65:HIS:CD2  | 2.48                     | 0.48              |
| 44:RY:19:LYS:HD2  | 44:RY:67:LEU:HD11 | 1.96                     | 0.48              |
| 44:YY:19:LYS:HB2  | 44:YY:20:TYR:H    | 1.34                     | 0.48              |
| 35:RP:16:ARG:HA   | 35:RP:16:ARG:HE   | 1.78                     | 0.48              |
| 45:RZ:118:GLN:HG2 | 45:RZ:172:ALA:HA  | 1.95                     | 0.48              |
| 1:QA:974:A:OP2    | 14:QN:41:ARG:NH1  | 2.46                     | 0.48              |
| 30:RG:104:GLU:HG2 | 50:R4:23:GLU:HG3  | 1.94                     | 0.48              |
| 2:XB:54:THR:HG21  | 2:XB:201:ILE:HD11 | 1.96                     | 0.48              |
| 28:YE:50:GLY:HA2  | 28:YE:74:PRO:HG3  | 1.94                     | 0.48              |
| 26:YB:44:G:H1'    | 26:YB:47:C:H42    | 1.79                     | 0.48              |
| 5:XE:7:GLU:HG2    | 5:XE:112:LEU:HD22 | 1.95                     | 0.48              |
| 1:QA:560:U:O2'    | 1:QA:561:U:OP2    | 2.27                     | 0.48              |
| 25:YA:748:G:OP1   | 25:YA:2612:C:N4   | 2.46                     | 0.48              |
| 31:YH:124:GLU:HB2 | 31:YH:132:ARG:HG3 | 1.95                     | 0.48              |
| 29:RF:78:ILE:HA   | 29:RF:83:PHE:CD1  | 2.48                     | 0.48              |
| 10:XJ:86:MET:HG2  | 10:XJ:87:THR:HG23 | 1.95                     | 0.48              |
| 25:RA:2267:A:H5'' | 25:RA:2268:A:H5'  | 1.94                     | 0.48              |
| 1:XA:33:A:H2'     | 1:XA:34:C:C6      | 2.49                     | 0.48              |
| 6:XF:50:TYR:CE1   | 18:XR:77:GLY:HA2  | 2.48                     | 0.48              |
| 18:XR:22:VAL:O    | 18:XR:24:ALA:N    | 2.42                     | 0.48              |
| 42:YW:64:MET:HE3  | 42:YW:109:GLU:HG3 | 1.96                     | 0.48              |
| 1:XA:31:G:O2'     | 1:XA:48:C:N4      | 2.46                     | 0.48              |
| 13:XM:9:ILE:HG12  | 13:XM:10:PRO:CD   | 2.43                     | 0.48              |
| 25:YA:2422:A:H4'  | 25:YA:2423:U:OP1  | 2.13                     | 0.48              |
| 28:RE:47:VAL:O    | 28:RE:48:GLN:O    | 2.30                     | 0.48              |
| 1:QA:114:U:H1'    | 1:QA:353:A:H1'    | 1.95                     | 0.48              |
| 1:QA:1347:G:O2'   | 1:QA:1348:U:OP2   | 2.30                     | 0.48              |
| 29:YF:7:TYR:HB3   | 29:YF:18:ARG:HB2  | 1.96                     | 0.48              |
| 4:XD:3:ARG:HE     | 4:XD:118:ARG:NE   | 2.11                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:1171:G:O2'  | 25:RA:1173:G:O5'   | 2.29                     | 0.48              |
| 1:XA:542:G:H5'    | 4:XD:41:GLY:HA3    | 1.94                     | 0.48              |
| 44:RY:62:GLU:CD   | 44:RY:63:LYS:H     | 2.17                     | 0.48              |
| 33:YN:30:ILE:HG21 | 33:YN:120:LEU:HD13 | 1.95                     | 0.48              |
| 25:YA:1930:G:HO2' | 25:YA:1931:U:P     | 2.31                     | 0.48              |
| 1:QA:1068:G:N2    | 1:QA:1191:A:N3     | 2.59                     | 0.48              |
| 52:Y6:34:LEU:HD11 | 52:Y6:50:ARG:HH21  | 1.78                     | 0.48              |
| 25:YA:1094:U:O2'  | 25:YA:1096:A:OP1   | 2.29                     | 0.48              |
| 54:Y8:31:HIS:CG   | 54:Y8:32:LEU:N     | 2.81                     | 0.48              |
| 25:RA:1062:G:H2'  | 25:RA:1063:G:C8    | 2.49                     | 0.48              |
| 1:QA:376:G:H5''   | 16:QP:5:ARG:HB2    | 1.94                     | 0.48              |
| 25:YA:1999:C:H4'  | 25:YA:2723:C:O2    | 2.13                     | 0.48              |
| 8:QH:85:ARG:HG2   | 8:QH:88:LYS:HG2    | 1.95                     | 0.48              |
| 25:YA:2823:A:OP1  | 28:YE:159:HIS:NE2  | 2.46                     | 0.48              |
| 25:RA:1952:A:C6   | 34:RO:22:ILE:HD12  | 2.48                     | 0.48              |
| 25:YA:2150:U:H2'  | 25:YA:2151:G:C8    | 2.48                     | 0.48              |
| 25:YA:1870:C:H2'  | 25:YA:1871:A:O4'   | 2.13                     | 0.48              |
| 25:RA:2106:G:N2   | 25:RA:2183:C:O2    | 2.47                     | 0.48              |
| 22:XW:66:C:H2'    | 22:XW:67:C:C6      | 2.49                     | 0.48              |
| 10:QJ:23:ILE:HG23 | 10:QJ:85:LEU:HD22  | 1.95                     | 0.48              |
| 25:YA:2725:A:O2'  | 25:YA:2726:U:OP2   | 2.24                     | 0.48              |
| 1:XA:1055:A:H4'   | 3:XC:161:GLU:CD    | 2.33                     | 0.48              |
| 25:YA:635:C:O2'   | 25:YA:639:U:OP1    | 2.31                     | 0.48              |
| 53:Y7:16:HIS:HB2  | 53:Y7:44:PRO:HG2   | 1.96                     | 0.48              |
| 28:RE:151:TYR:HD2 | 28:RE:154:LYS:HZ2  | 1.59                     | 0.48              |
| 36:RQ:116:GLU:O   | 36:RQ:120:ILE:HG12 | 2.13                     | 0.48              |
| 1:XA:1015:A:H2'   | 1:XA:1016:A:C8     | 2.49                     | 0.48              |
| 1:QA:950:U:H2'    | 1:QA:951:G:C8      | 2.49                     | 0.48              |
| 25:YA:986:C:H2'   | 25:YA:987:G:H5'    | 1.96                     | 0.48              |
| 41:RV:10:LYS:NZ   | 41:RV:23:GLU:OE1   | 2.46                     | 0.48              |
| 1:QA:316:G:O5'    | 1:QA:316:G:H8      | 1.97                     | 0.48              |
| 25:YA:570:G:H2'   | 25:YA:2030:A:C5    | 2.47                     | 0.48              |
| 1:XA:501:C:OP1    | 12:XL:117:ARG:NH2  | 2.41                     | 0.48              |
| 11:XK:54:ARG:HH11 | 11:XK:54:ARG:CG    | 2.25                     | 0.48              |
| 25:YA:2016:U:H1'  | 51:Y5:6:VAL:HG12   | 1.95                     | 0.48              |
| 52:Y6:15:GLU:OE2  | 52:Y6:44:ARG:NH1   | 2.43                     | 0.48              |
| 25:YA:2693:A:H2'  | 25:YA:2694:G:H8    | 1.79                     | 0.48              |
| 25:RA:360:G:H2'   | 25:RA:361:G:H8     | 1.79                     | 0.48              |
| 1:QA:738:C:OP1    | 6:QF:92:LYS:HD2    | 2.13                     | 0.48              |
| 1:QA:1237:C:N4    | 1:QA:1336:C:O2     | 2.46                     | 0.48              |
| 19:QS:42:PRO:HG3  | 50:R4:60:GLN:HE21  | 1.79                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:1374:G:H2'  | 25:RA:1375:C:C6    | 2.48                     | 0.48              |
| 1:QA:694:A:O2'    | 22:QW:38:A:O2'     | 2.29                     | 0.48              |
| 25:YA:1385:G:O2'  | 25:YA:1396:U:O2    | 2.32                     | 0.48              |
| 41:RV:98:GLU:OE2  | 41:RV:100:ARG:NH1  | 2.47                     | 0.48              |
| 22:QW:67:C:H2'    | 22:QW:68:C:C6      | 2.49                     | 0.48              |
| 1:XA:1422:G:O3'   | 34:YO:49:ARG:NH1   | 2.44                     | 0.48              |
| 25:RA:2732:G:H3'  | 25:RA:2733:A:H5'   | 1.95                     | 0.48              |
| 34:RO:4:PRO:O     | 34:RO:5:GLN:HB2    | 2.13                     | 0.48              |
| 27:RD:145:VAL:HB  | 27:RD:155:LEU:HB2  | 1.95                     | 0.48              |
| 12:QL:27:LEU:HD13 | 12:QL:33:ARG:HB2   | 1.95                     | 0.48              |
| 34:YO:73:ASP:OD1  | 39:YT:32:TYR:OH    | 2.30                     | 0.48              |
| 32:RI:57:ARG:HA   | 32:RI:60:GLU:HB3   | 1.95                     | 0.48              |
| 1:XA:1218:C:H2'   | 1:XA:1219:U:C6     | 2.48                     | 0.48              |
| 31:RH:8:PRO:O     | 31:RH:9:ILE:CB     | 2.61                     | 0.48              |
| 19:QS:38:SER:O    | 19:QS:70:LYS:HB3   | 2.14                     | 0.48              |
| 1:QA:1029:C:H2'   | 1:QA:1030:C:C6     | 2.48                     | 0.48              |
| 40:YU:50:ARG:HH11 | 41:YV:72:VAL:HG11  | 1.78                     | 0.48              |
| 2:XB:18:GLY:HA2   | 2:XB:40:HIS:O      | 2.13                     | 0.48              |
| 39:YT:39:ARG:NH2  | 39:YT:41:ARG:HG2   | 2.28                     | 0.48              |
| 25:YA:1578:U:C2'  | 25:YA:1579:A:H5'   | 2.44                     | 0.48              |
| 36:RQ:34:LEU:HD11 | 36:RQ:129:THR:HB   | 1.96                     | 0.48              |
| 1:XA:1062:U:H2'   | 1:XA:1063:C:C6     | 2.49                     | 0.48              |
| 1:QA:73:G:H1      | 1:QA:96:U:H3       | 1.62                     | 0.48              |
| 41:YV:49:THR:HG22 | 41:YV:50:PRO:HG3   | 1.93                     | 0.48              |
| 44:RY:84:ARG:NH2  | 44:RY:97:ARG:HB2   | 2.28                     | 0.48              |
| 14:XN:41:ARG:NE   | 14:XN:42:ILE:HD11  | 2.28                     | 0.48              |
| 52:Y6:28:ARG:HB2  | 52:Y6:31:PRO:HB2   | 1.96                     | 0.48              |
| 1:XA:1399:C:C2    | 1:XA:1502:A:N6     | 2.81                     | 0.48              |
| 25:YA:363:G:H5'   | 25:YA:363(A):A:OP2 | 2.14                     | 0.48              |
| 25:RA:1698:A:C8   | 25:RA:1700:A:O4'   | 2.66                     | 0.48              |
| 1:QA:1061:G:OP2   | 3:QC:3:ASN:ND2     | 2.43                     | 0.48              |
| 25:YA:1203:G:H5'  | 35:YP:3:LEU:HD12   | 1.96                     | 0.48              |
| 39:RT:26:ASP:HB2  | 39:RT:91:ARG:HA    | 1.96                     | 0.48              |
| 9:XI:20:ARG:O     | 9:XI:60:ASP:N      | 2.46                     | 0.48              |
| 25:RA:1085:A:H2'  | 25:RA:1086:A:C8    | 2.49                     | 0.48              |
| 3:XC:23:TYR:CD2   | 10:XJ:10:GLY:HA2   | 2.49                     | 0.48              |
| 27:YD:97:TYR:HB3  | 27:YD:99:ASP:OD1   | 2.13                     | 0.48              |
| 1:XA:901:A:C5     | 1:XA:902:G:H1'     | 2.49                     | 0.48              |
| 20:QT:26:ASN:HB3  | 20:QT:71:THR:OG1   | 2.14                     | 0.48              |
| 41:RV:38:LEU:HD12 | 41:RV:55:ALA:HB1   | 1.95                     | 0.48              |
| 1:XA:520:A:OP1    | 12:XL:52:LEU:HB2   | 2.14                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:YA:2884:U:O2    | 51:Y5:52:TYR:OH     | 2.32                     | 0.48              |
| 25:RA:139(A):G:H22 | 43:RX:44:GLU:CD     | 2.16                     | 0.48              |
| 25:YA:1141:U:H4'   | 25:YA:1142(A):A:O4' | 2.13                     | 0.48              |
| 45:RZ:52:SER:O     | 45:RZ:54:HIS:N      | 2.46                     | 0.48              |
| 1:XA:445:G:H2'     | 1:XA:446:G:H8       | 1.79                     | 0.48              |
| 36:YQ:138:ASP:OD2  | 36:YQ:138:ASP:N     | 2.46                     | 0.48              |
| 20:XT:14:LYS:HA    | 20:XT:17:ARG:HE     | 1.78                     | 0.48              |
| 25:YA:1725:G:O6    | 25:YA:1735:C:N4     | 2.34                     | 0.48              |
| 1:QA:193:C:H2'     | 1:QA:194:C:C6       | 2.49                     | 0.48              |
| 32:RI:98:ALA:HA    | 32:RI:109:ILE:HD11  | 1.95                     | 0.48              |
| 13:XM:10:PRO:O     | 13:XM:45:VAL:HG11   | 2.14                     | 0.48              |
| 25:RA:2447:G:H4'   | 25:RA:2448:A:O5'    | 2.14                     | 0.48              |
| 25:RA:1548:C:N3    | 25:RA:1549:C:N4     | 2.61                     | 0.48              |
| 1:QA:1347:G:O2'    | 9:QI:109:VAL:HA     | 2.14                     | 0.48              |
| 12:XL:53:ARG:NH2   | 12:XL:92:ASP:OD2    | 2.33                     | 0.48              |
| 1:QA:974:A:O2'     | 1:QA:976:G:H5''     | 2.13                     | 0.48              |
| 22:XW:18:G:H1'     | 22:XW:58:A:C2       | 2.48                     | 0.48              |
| 1:XA:265:G:H5'     | 17:XQ:64:PRO:O      | 2.12                     | 0.48              |
| 31:RH:51:ARG:HG3   | 31:RH:51:ARG:H      | 1.32                     | 0.48              |
| 16:QP:71:ARG:HG3   | 16:QP:80:PHE:CE1    | 2.47                     | 0.48              |
| 28:YE:68:ALA:O     | 28:YE:70:ALA:N      | 2.47                     | 0.48              |
| 28:YE:75:VAL:O     | 28:YE:77:ILE:N      | 2.47                     | 0.48              |
| 1:XA:403:C:H2'     | 1:XA:404:U:C6       | 2.48                     | 0.48              |
| 25:RA:545:C:H2'    | 25:RA:547:A:O4'     | 2.14                     | 0.48              |
| 25:YA:1274:A:N3    | 25:YA:1297:C:H1'    | 2.29                     | 0.48              |
| 36:YQ:116:GLU:O    | 36:YQ:120:ILE:HG12  | 2.13                     | 0.48              |
| 39:RT:105:LEU:HD13 | 39:RT:109:GLU:HG3   | 1.95                     | 0.48              |
| 1:XA:503:C:OP2     | 12:XL:116:SER:HB3   | 2.13                     | 0.48              |
| 25:RA:362:U:H5'    | 25:RA:363:G:OP2     | 2.13                     | 0.48              |
| 1:XA:1495:U:O2'    | 25:YA:1919:A:N1     | 2.39                     | 0.48              |
| 1:QA:4:U:O2        | 8:QH:102:ARG:NH1    | 2.47                     | 0.48              |
| 1:XA:1175:G:H2'    | 1:XA:1176:A:C8      | 2.48                     | 0.48              |
| 22:QW:17:C:H2'     | 22:QW:17(A):U:C6    | 2.49                     | 0.48              |
| 25:YA:1278:A:H2'   | 25:YA:1279:G:H8     | 1.79                     | 0.48              |
| 11:XK:34:ASP:HB3   | 11:XK:40:ILE:HD11   | 1.96                     | 0.48              |
| 33:RN:17:ASP:OD2   | 33:RN:56:ASN:ND2    | 2.29                     | 0.48              |
| 54:R8:33:ASN:OD1   | 54:R8:33:ASN:N      | 2.47                     | 0.48              |
| 22:XV:53:G:H2'     | 22:XV:54:U:H5'      | 1.96                     | 0.48              |
| 29:YF:25:PRO:HD3   | 29:YF:115:ALA:HB1   | 1.96                     | 0.48              |
| 3:QC:20:SER:HB2    | 3:QC:40:ARG:HH12    | 1.78                     | 0.48              |
| 1:XA:674:G:H2'     | 1:XA:675:A:C8       | 2.49                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:RD:35:LYS:HZ1  | 27:RD:65:ILE:HA   | 1.78                     | 0.48              |
| 25:RA:78:A:H2'    | 25:RA:79:G:C8     | 2.49                     | 0.48              |
| 25:YA:2887:U:H2'  | 25:YA:2888:C:H6   | 1.77                     | 0.48              |
| 11:QK:30:VAL:HG21 | 11:QK:65:ALA:HA   | 1.94                     | 0.48              |
| 41:RV:58:VAL:HB   | 41:RV:98:GLU:HB2  | 1.95                     | 0.48              |
| 1:XA:580:U:H2'    | 1:XA:581:G:O4'    | 2.13                     | 0.48              |
| 25:RA:946:G:H2'   | 25:RA:947:G:C8    | 2.49                     | 0.48              |
| 25:RA:729:G:H2'   | 25:RA:1775:U:H1'  | 1.96                     | 0.48              |
| 25:RA:1149:G:H2'  | 25:RA:1150:C:C6   | 2.49                     | 0.48              |
| 1:QA:262:A:C6     | 1:QA:263:A:C6     | 3.02                     | 0.48              |
| 1:QA:1457:G:OP1   | 20:QT:39:LYS:NZ   | 2.39                     | 0.48              |
| 25:RA:2654:A:O2'  | 25:RA:2655:G:H4'  | 2.14                     | 0.48              |
| 25:RA:1268:A:H2'  | 25:RA:1269:A:O4'  | 2.13                     | 0.48              |
| 1:XA:1348:U:H3    | 1:XA:1374:A:H2    | 1.59                     | 0.48              |
| 28:YE:87:GLU:HG3  | 28:YE:89:ASP:H    | 1.78                     | 0.48              |
| 25:RA:921:G:H4'   | 25:RA:2269:A:C5   | 2.49                     | 0.48              |
| 25:YA:185:U:H4'   | 25:YA:218:A:H4'   | 1.95                     | 0.48              |
| 1:XA:1068:G:H8    | 1:XA:1068:G:OP2   | 1.96                     | 0.48              |
| 1:QA:115:G:H4'    | 1:QA:116:A:O5'    | 2.13                     | 0.48              |
| 28:RE:33:VAL:HG23 | 28:RE:47:VAL:HG13 | 1.96                     | 0.47              |
| 25:RA:2701:C:C3'  | 25:RA:2702:U:H5'' | 2.25                     | 0.47              |
| 19:XS:36:ARG:NH2  | 19:XS:73:GLU:OE2  | 2.45                     | 0.47              |
| 25:RA:996:A:H4'   | 40:RU:92:ARG:CZ   | 2.44                     | 0.47              |
| 25:YA:607:U:OP1   | 29:YF:102:PRO:HA  | 2.14                     | 0.47              |
| 1:QA:717:C:H4'    | 11:QK:117:ASN:HB3 | 1.96                     | 0.47              |
| 24:XY:91:TYR:C    | 24:XY:91:TYR:CD2  | 2.86                     | 0.47              |
| 19:XS:44:MET:HG2  | 19:XS:47:HIS:NE2  | 2.28                     | 0.47              |
| 19:XS:66:MET:HA   | 19:XS:69:HIS:HD2  | 1.79                     | 0.47              |
| 27:RD:35:LYS:NZ   | 27:RD:64:ILE:O    | 2.43                     | 0.47              |
| 25:RA:686:G:N2    | 25:RA:788:A:H61   | 2.12                     | 0.47              |
| 25:RA:2328:A:H2'  | 25:RA:2329:G:C8   | 2.49                     | 0.47              |
| 28:YE:8:LYS:HB3   | 28:YE:193:GLY:N   | 2.29                     | 0.47              |
| 25:RA:2144:U:H4'  | 25:RA:2145:C:OP1  | 2.14                     | 0.47              |
| 1:XA:1234:C:H4'   | 1:XA:1364:U:H1'   | 1.96                     | 0.47              |
| 25:RA:2696:U:H2'  | 25:RA:2697:G:C8   | 2.49                     | 0.47              |
| 25:YA:2695:C:H2'  | 25:YA:2696:U:C6   | 2.48                     | 0.47              |
| 37:YR:52:ILE:HD13 | 37:YR:79:LEU:HD21 | 1.95                     | 0.47              |
| 3:QC:130:VAL:O    | 3:QC:134:ILE:HG12 | 2.13                     | 0.47              |
| 28:RE:116:VAL:O   | 28:RE:117:MET:HB3 | 2.14                     | 0.47              |
| 18:XR:26:LEU:HD22 | 18:XR:39:VAL:HG13 | 1.96                     | 0.47              |
| 25:YA:515:A:H1'   | 25:YA:581:C:H1'   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:YH:38:SER:O    | 31:YH:40:GLU:N     | 2.47                     | 0.47              |
| 25:YA:1188:U:H4'  | 41:YV:79:VAL:HG12  | 1.95                     | 0.47              |
| 44:RY:75:ILE:HG13 | 44:RY:80:GLY:H     | 1.79                     | 0.47              |
| 25:RA:55:G:H2'    | 25:RA:56:A:H8      | 1.79                     | 0.47              |
| 25:YA:642:G:H21   | 25:YA:646:A:H2     | 1.59                     | 0.47              |
| 3:QC:66:VAL:HG13  | 3:QC:101:LEU:HA    | 1.96                     | 0.47              |
| 28:YE:130:GLY:O   | 28:YE:131:ALA:HB3  | 2.14                     | 0.47              |
| 29:YF:24:LEU:CD1  | 29:YF:25:PRO:HD2   | 2.44                     | 0.47              |
| 10:QJ:51:ARG:HB2  | 10:QJ:60:ARG:HA    | 1.95                     | 0.47              |
| 10:QJ:51:ARG:HE   | 10:QJ:61:GLU:HB2   | 1.78                     | 0.47              |
| 4:QD:15:GLU:O     | 4:QD:17:VAL:N      | 2.46                     | 0.47              |
| 25:YA:2645:G:H3'  | 25:YA:2646:C:H5'   | 1.96                     | 0.47              |
| 19:QS:45:VAL:O    | 19:QS:62:ILE:HB    | 2.14                     | 0.47              |
| 26:YB:14:U:O2'    | 26:YB:15:A:OP1     | 2.31                     | 0.47              |
| 1:XA:1127:G:H1'   | 1:XA:1280:A:C6     | 2.48                     | 0.47              |
| 39:YT:26:ASP:HB2  | 39:YT:90:GLN:O     | 2.14                     | 0.47              |
| 25:RA:2287:A:N6   | 25:RA:2344:U:H3    | 2.12                     | 0.47              |
| 1:QA:1300:G:HO2'  | 1:QA:1301:U:H5     | 1.52                     | 0.47              |
| 28:YE:200:GLU:HG2 | 28:YE:201:THR:H    | 1.79                     | 0.47              |
| 25:YA:1858:G:H8   | 25:YA:1858:G:OP2   | 1.97                     | 0.47              |
| 25:RA:300:A:H2'   | 25:RA:334:C:H1'    | 1.96                     | 0.47              |
| 1:QA:1337:G:H5''  | 1:QA:1338:G:OP1    | 2.14                     | 0.47              |
| 25:YA:197:A:N6    | 25:YA:2430:A:H2'   | 2.27                     | 0.47              |
| 1:XA:1217:C:OP1   | 14:YN:9:LYS:HD2    | 2.14                     | 0.47              |
| 33:RN:63:THR:O    | 33:RN:66:LYS:HG3   | 2.13                     | 0.47              |
| 25:RA:2296:U:OP2  | 38:RS:9:ARG:NH1    | 2.45                     | 0.47              |
| 41:YV:29:PRO:HA   | 41:YV:61:VAL:HG13  | 1.96                     | 0.47              |
| 4:QD:178:VAL:O    | 4:QD:180:GLY:N     | 2.45                     | 0.47              |
| 25:RA:1831:G:H2'  | 25:RA:1832:C:C6    | 2.50                     | 0.47              |
| 45:YZ:103:ARG:HB3 | 45:YZ:104:PHE:H    | 1.47                     | 0.47              |
| 1:QA:1347:G:C6    | 9:QI:107:ARG:NH2   | 2.82                     | 0.47              |
| 13:XM:99:ARG:O    | 13:XM:101:GLN:N    | 2.47                     | 0.47              |
| 50:Y4:58:ARG:NH2  | 50:Y4:62:ARG:HG3   | 2.29                     | 0.47              |
| 25:RA:1375:C:H2'  | 25:RA:1376:C:C6    | 2.49                     | 0.47              |
| 37:YR:78:LYS:HE2  | 37:YR:83:ILE:HD11  | 1.95                     | 0.47              |
| 25:RA:1550:C:O5'  | 25:RA:1550:C:H6    | 1.97                     | 0.47              |
| 10:XJ:54:PHE:CG   | 10:XJ:55:LYS:N     | 2.83                     | 0.47              |
| 25:YA:1141:U:O2   | 25:YA:1142(A):A:N6 | 2.47                     | 0.47              |
| 20:XT:53:LEU:HB3  | 20:XT:102:GLY:HA3  | 1.94                     | 0.47              |
| 45:YZ:48:PHE:HE2  | 45:YZ:71:VAL:HG21  | 1.80                     | 0.47              |
| 25:RA:1047:G:H2'  | 25:RA:1110:G:N1    | 2.30                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:XJ:27:ALA:HB2   | 10:XJ:85:LEU:HD11  | 1.94                     | 0.47              |
| 50:Y4:14:ILE:HG23  | 50:Y4:21:VAL:HG23  | 1.96                     | 0.47              |
| 1:XA:1096:C:H2'    | 1:XA:1097:C:C6     | 2.50                     | 0.47              |
| 34:RO:35:VAL:HG11  | 34:RO:103:ALA:HB3  | 1.96                     | 0.47              |
| 1:XA:793:U:H5'     | 1:XA:794:A:O5'     | 2.13                     | 0.47              |
| 25:YA:2610:C:H4'   | 25:YA:2611:U:OP2   | 2.13                     | 0.47              |
| 41:RV:64:HIS:CE1   | 41:RV:92:THR:HG1   | 2.31                     | 0.47              |
| 25:RA:271(C):C:H2' | 25:RA:271(D):G:C8  | 2.49                     | 0.47              |
| 43:RX:43:VAL:HG23  | 43:RX:51:VAL:HG21  | 1.97                     | 0.47              |
| 25:RA:2098:U:H3    | 25:RA:2191:G:H1    | 1.62                     | 0.47              |
| 1:QA:909:A:H2'     | 1:QA:910:C:O4'     | 2.14                     | 0.47              |
| 44:RY:40:GLU:OE2   | 44:RY:40:GLU:N     | 2.46                     | 0.47              |
| 1:QA:57:G:H2'      | 1:QA:58:C:C6       | 2.50                     | 0.47              |
| 1:XA:742:G:OP2     | 15:XO:35:ARG:NH2   | 2.47                     | 0.47              |
| 45:YZ:51:ALA:HB1   | 45:YZ:57:ILE:HD11  | 1.97                     | 0.47              |
| 8:QH:64:LYS:HG2    | 8:QH:79:VAL:HG21   | 1.96                     | 0.47              |
| 1:XA:975:A:H61     | 10:XJ:48:THR:HB    | 1.78                     | 0.47              |
| 31:YH:9:ILE:HG23   | 31:YH:51:ARG:HA    | 1.95                     | 0.47              |
| 29:YF:4:VAL:HG11   | 29:YF:17:ARG:HE    | 1.78                     | 0.47              |
| 25:YA:2405:G:OP1   | 35:YP:77:ARG:NH2   | 2.46                     | 0.47              |
| 25:YA:264:C:O2'    | 25:YA:265:A:H2'    | 2.14                     | 0.47              |
| 27:RD:92:ILE:HD12  | 27:RD:104:TYR:CD2  | 2.49                     | 0.47              |
| 1:XA:1327:C:H2'    | 1:XA:1328:C:C6     | 2.50                     | 0.47              |
| 25:YA:859:G:O2'    | 25:YA:860:U:P      | 2.72                     | 0.47              |
| 28:YE:120:TRP:CD2  | 28:YE:155:LYS:HD3  | 2.48                     | 0.47              |
| 1:QA:1521:G:H2'    | 1:QA:1522:U:C6     | 2.49                     | 0.47              |
| 22:QW:36:U:H2'     | 22:QW:37:A:C8      | 2.49                     | 0.47              |
| 8:QH:102:ARG:H     | 8:QH:102:ARG:HG3   | 1.41                     | 0.47              |
| 43:RX:40:LYS:HG3   | 43:RX:51:VAL:HB    | 1.97                     | 0.47              |
| 9:XI:117:HIS:CD2   | 9:XI:123:PRO:HA    | 2.49                     | 0.47              |
| 35:YP:84:ASN:HA    | 35:YP:115:LEU:O    | 2.14                     | 0.47              |
| 38:YS:3:ARG:HD3    | 38:YS:4:LEU:HB2    | 1.96                     | 0.47              |
| 22:QV:50:U:H2'     | 22:QV:51:C:C6      | 2.49                     | 0.47              |
| 7:XG:18:TYR:HD2    | 7:XG:59:LEU:HD22   | 1.79                     | 0.47              |
| 25:RA:1221(A):C:C2 | 25:RA:1229:G:C2    | 3.03                     | 0.47              |
| 3:XC:116:VAL:HG21  | 3:XC:202:ILE:HD11  | 1.96                     | 0.47              |
| 36:RQ:21:THR:OG1   | 36:RQ:23:GLY:O     | 2.32                     | 0.47              |
| 25:YA:1427:A:H4'   | 25:YA:1428:C:O5'   | 2.13                     | 0.47              |
| 27:RD:131:LEU:HB2  | 27:RD:136:ILE:HD11 | 1.97                     | 0.47              |
| 25:RA:1174:A:H62   | 25:RA:1177:A:H4'   | 1.80                     | 0.47              |
| 25:YA:1544:C:C2'   | 25:YA:1544:C:O2    | 2.62                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:RB:7:G:N2      | 38:RS:38:GLN:OE1   | 2.39                     | 0.47              |
| 33:YN:95:PRO:O    | 33:YN:98:VAL:HG22  | 2.14                     | 0.47              |
| 3:XC:32:LEU:HD22  | 3:XC:59:ARG:NH1    | 2.30                     | 0.47              |
| 48:Y2:15:LYS:HE3  | 48:Y2:67:LYS:HE2   | 1.95                     | 0.47              |
| 25:RA:2689:U:H4'  | 25:RA:2690:C:H5'   | 1.96                     | 0.47              |
| 41:YV:85:LYS:HD2  | 41:YV:86:GLY:H     | 1.79                     | 0.47              |
| 1:QA:1147:C:H2'   | 9:QI:16:ARG:HD3    | 1.95                     | 0.47              |
| 52:R6:9:LEU:HD22  | 52:R6:10:LEU:H     | 1.80                     | 0.47              |
| 36:RQ:83:MET:HB2  | 46:R0:7:LEU:HD13   | 1.96                     | 0.47              |
| 26:YB:45:A:OP2    | 30:YG:96:ARG:NH1   | 2.46                     | 0.47              |
| 1:XA:1137:C:H5'   | 1:XA:1138:G:C4     | 2.49                     | 0.47              |
| 25:RA:859:G:O2'   | 25:RA:860:U:C6     | 2.67                     | 0.47              |
| 1:XA:1118:C:H2'   | 1:XA:1119:C:C6     | 2.50                     | 0.47              |
| 38:YS:7:TYR:CZ    | 38:YS:91:PRO:HG3   | 2.49                     | 0.47              |
| 25:RA:774:A:H2    | 25:RA:787:U:O2'    | 1.97                     | 0.47              |
| 25:RA:2481:G:O2'  | 25:RA:2482:G:O5'   | 2.30                     | 0.47              |
| 1:XA:1403:C:H1'   | 1:XA:1500:A:N1     | 2.29                     | 0.47              |
| 12:QL:127:GLU:O   | 12:QL:129:ALA:N    | 2.48                     | 0.47              |
| 25:YA:2155:G:H2'  | 25:YA:2156:G:O4'   | 2.14                     | 0.47              |
| 1:QA:1166:G:N2    | 1:QA:1170:A:OP2    | 2.44                     | 0.47              |
| 25:YA:1882:C:H5'  | 25:YA:1883:G:OP2   | 2.15                     | 0.47              |
| 1:XA:719:C:O2'    | 18:XR:49:LYS:HB3   | 2.14                     | 0.47              |
| 11:QK:22:HIS:HB3  | 11:QK:29:ILE:HG12  | 1.97                     | 0.47              |
| 25:YA:1688:U:O2   | 25:YA:1700:A:H5'   | 2.14                     | 0.47              |
| 25:RA:389:G:H22   | 35:RP:72:PRO:HD3   | 1.79                     | 0.47              |
| 25:RA:1198:U:H2'  | 25:RA:1199:U:C6    | 2.50                     | 0.47              |
| 25:YA:270(E):G:H1 | 25:YA:270(U):C:H42 | 1.61                     | 0.47              |
| 25:YA:468:G:N7    | 53:Y7:39:ARG:NH2   | 2.56                     | 0.47              |
| 25:RA:2786:U:C5'  | 28:RE:66:HIS:HD2   | 2.27                     | 0.47              |
| 41:RV:85:LYS:HG3  | 41:RV:87:HIS:N     | 2.29                     | 0.47              |
| 1:QA:1347:G:H4'   | 1:QA:1348:U:H6     | 1.79                     | 0.47              |
| 9:QI:28:VAL:HG22  | 9:QI:29:ASN:N      | 2.30                     | 0.47              |
| 3:XC:76:VAL:HG13  | 3:XC:84:ILE:HG13   | 1.97                     | 0.47              |
| 21:XU:9:ARG:HH21  | 21:XU:10:ARG:HH21  | 1.61                     | 0.47              |
| 52:Y6:42:TRP:HD1  | 52:Y6:44:ARG:HG2   | 1.79                     | 0.47              |
| 13:QM:118:ALA:HB2 | 22:QV:29:G:H5'     | 1.96                     | 0.47              |
| 1:QA:1008:C:H3'   | 1:QA:1009:G:H5''   | 1.95                     | 0.47              |
| 2:QB:97:TRP:CH2   | 2:QB:173:ALA:HA    | 2.50                     | 0.47              |
| 33:RN:39:ARG:HH21 | 33:RN:41:ASP:CB    | 2.27                     | 0.47              |
| 25:YA:2591:C:H2'  | 25:YA:2592:G:H8    | 1.78                     | 0.47              |
| 1:XA:620:C:C2     | 4:XD:135:LEU:HG    | 2.49                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1869:G:H5'   | 25:YA:1870:C:OP2   | 2.14                     | 0.47              |
| 45:YZ:127:LYS:O    | 45:YZ:162:GLU:HG2  | 2.14                     | 0.47              |
| 25:YA:576:U:H2'    | 25:YA:577:G:C8     | 2.49                     | 0.47              |
| 29:YF:157:VAL:HB   | 29:YF:194:MET:HB3  | 1.97                     | 0.47              |
| 10:XJ:30:SER:OG    | 10:XJ:81:THR:HG22  | 2.15                     | 0.47              |
| 25:YA:491:G:H2'    | 25:YA:492:A:C8     | 2.49                     | 0.47              |
| 38:YS:30:ARG:HH21  | 38:YS:92:TYR:HD1   | 1.63                     | 0.47              |
| 30:YG:107:LEU:HD11 | 30:YG:178:PHE:CE1  | 2.49                     | 0.47              |
| 1:XA:908:A:H2'     | 1:XA:909:A:H8      | 1.78                     | 0.47              |
| 33:YN:93:THR:HB    | 33:YN:94:HIS:CE1   | 2.50                     | 0.47              |
| 22:QW:20:U:H3'     | 22:QW:21:A:H5''    | 1.94                     | 0.47              |
| 38:RS:108:GLY:O    | 38:RS:110:LEU:N    | 2.48                     | 0.47              |
| 10:XJ:48:THR:HG22  | 10:XJ:60:ARG:HD2   | 1.97                     | 0.47              |
| 28:RE:35:GLN:HE22  | 28:RE:37:ARG:NH2   | 2.12                     | 0.47              |
| 23:XX:12:A:H5'     | 23:XX:13:A:OP2     | 2.15                     | 0.47              |
| 45:RZ:118:GLN:HE21 | 45:RZ:174:VAL:HA   | 1.78                     | 0.47              |
| 22:QW:19:G:C6      | 25:RA:2112:G:C2    | 3.03                     | 0.47              |
| 10:QJ:49:VAL:HG22  | 14:QN:41:ARG:HB2   | 1.95                     | 0.47              |
| 31:YH:54:ARG:H     | 31:YH:54:ARG:HD3   | 1.80                     | 0.47              |
| 25:YA:483:A:C5'    | 44:YY:49:VAL:HA    | 2.45                     | 0.47              |
| 25:RA:49:A:H4'     | 25:RA:50:U:H5''    | 1.97                     | 0.47              |
| 1:XA:1126:U:O2     | 1:XA:1280:A:H5''   | 2.15                     | 0.47              |
| 34:YO:87:ILE:HG21  | 34:YO:91:LEU:HD13  | 1.95                     | 0.47              |
| 25:RA:582:G:H2'    | 25:RA:583:G:C8     | 2.50                     | 0.47              |
| 31:YH:150:ALA:O    | 31:YH:152:ARG:N    | 2.47                     | 0.47              |
| 46:Y0:27:GLU:HB2   | 46:Y0:69:PHE:HD1   | 1.80                     | 0.47              |
| 25:RA:708:C:H42    | 25:RA:723:G:H1     | 1.63                     | 0.47              |
| 45:RZ:130:PRO:O    | 45:RZ:133:ILE:HD11 | 2.14                     | 0.47              |
| 46:Y0:4:LYS:HB2    | 46:Y0:5:LYS:HA     | 1.96                     | 0.47              |
| 25:RA:2286:A:H8    | 25:RA:2287:A:N6    | 2.13                     | 0.47              |
| 1:QA:1237:C:O2'    | 1:QA:1300:G:N2     | 2.41                     | 0.47              |
| 25:RA:2756:U:OP2   | 55:R9:19:ARG:NE    | 2.46                     | 0.47              |
| 25:RA:1416:G:H2'   | 25:RA:1417:C:C6    | 2.49                     | 0.47              |
| 25:RA:264:C:O2'    | 25:RA:265:A:H2'    | 2.15                     | 0.47              |
| 25:RA:876:C:H2'    | 25:RA:877:U:O4'    | 2.15                     | 0.47              |
| 1:QA:411:A:N6      | 1:QA:413:G:H21     | 2.13                     | 0.47              |
| 25:RA:2307:G:OP1   | 25:RA:2307:G:H8    | 1.97                     | 0.47              |
| 26:RB:79:C:H2'     | 26:RB:80:U:O4'     | 2.14                     | 0.47              |
| 25:RA:574:C:N3     | 28:RE:145:LYS:NZ   | 2.63                     | 0.47              |
| 30:YG:15:VAL:HG21  | 30:YG:176:LEU:HD23 | 1.96                     | 0.47              |
| 2:XB:82:ARG:HB3    | 2:XB:94:ASN:ND2    | 2.29                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:RI:2:LYS:HB2   | 32:RI:39:ALA:HB3   | 1.97                     | 0.47              |
| 25:YA:873:G:O2'   | 36:YQ:63:LYS:NZ    | 2.48                     | 0.47              |
| 28:RE:111:ARG:HA  | 37:RR:2:ARG:NH1    | 2.29                     | 0.47              |
| 5:QE:78:HIS:HD1   | 8:QH:104:ARG:HG3   | 1.78                     | 0.47              |
| 1:XA:1205:U:H4'   | 3:XC:195:VAL:HG21  | 1.96                     | 0.47              |
| 25:YA:593:G:C1'   | 54:Y8:4:MET:HE1    | 2.45                     | 0.47              |
| 33:YN:14:VAL:HA   | 33:YN:135:PRO:HD2  | 1.96                     | 0.47              |
| 1:XA:598:U:H4'    | 8:XH:94:TYR:CD2    | 2.49                     | 0.47              |
| 1:XA:181:G:O2'    | 1:XA:182:U:O5'     | 2.28                     | 0.47              |
| 5:QE:101:ILE:HD11 | 5:QE:119:LEU:HD23  | 1.97                     | 0.47              |
| 1:QA:1304:G:N1    | 1:QA:1332:A:OP2    | 2.42                     | 0.47              |
| 25:YA:137(A):G:H1 | 25:YA:141(A):C:H42 | 1.62                     | 0.47              |
| 25:YA:2120:G:H1   | 25:YA:2178:C:H42   | 1.62                     | 0.47              |
| 2:XB:21:ARG:HA    | 2:XB:39:ILE:H      | 1.78                     | 0.47              |
| 28:RE:73:GLU:HG3  | 28:RE:74:PRO:HD2   | 1.95                     | 0.47              |
| 27:YD:68:LYS:HB2  | 27:YD:70:TRP:CE2   | 2.49                     | 0.47              |
| 10:QJ:54:PHE:CG   | 10:QJ:55:LYS:N     | 2.83                     | 0.47              |
| 7:XG:129:GLU:HG2  | 7:XG:131:LYS:HZ2   | 1.80                     | 0.47              |
| 25:RA:931:G:H4'   | 49:R3:24:LYS:HE3   | 1.95                     | 0.47              |
| 30:RG:94:LEU:HD12 | 30:RG:99:MET:HA    | 1.95                     | 0.47              |
| 1:QA:204:U:O2'    | 1:QA:216:G:O4'     | 2.31                     | 0.47              |
| 25:RA:1766:U:H2'  | 25:RA:1767:C:H6    | 1.80                     | 0.47              |
| 45:YZ:119:GLU:OE1 | 45:YZ:122:ARG:NH2  | 2.44                     | 0.47              |
| 25:RA:2150:U:H2'  | 25:RA:2151:G:C8    | 2.49                     | 0.47              |
| 38:YS:10:ARG:O    | 38:YS:14:VAL:HG12  | 2.15                     | 0.47              |
| 1:QA:323:U:H2'    | 1:QA:324:G:O4'     | 2.15                     | 0.47              |
| 25:YA:2683:C:OP1  | 39:YT:53:ARG:NH2   | 2.47                     | 0.47              |
| 22:QW:56:C:H2'    | 22:QW:57:A:C8      | 2.50                     | 0.47              |
| 49:R3:38:GLU:HB3  | 49:R3:40:THR:HG23  | 1.97                     | 0.47              |
| 47:Y1:51:VAL:HG11 | 47:Y1:74:VAL:HG21  | 1.97                     | 0.47              |
| 50:Y4:46:GLN:HE21 | 50:Y4:48:ARG:HD3   | 1.80                     | 0.47              |
| 31:RH:32:GLU:HG2  | 31:RH:34:GLU:H     | 1.80                     | 0.47              |
| 7:XG:47:CYS:HB3   | 7:XG:58:PRO:HG3    | 1.96                     | 0.47              |
| 25:YA:2298:A:H2'  | 25:YA:2299:G:O4'   | 2.13                     | 0.47              |
| 31:RH:76:VAL:O    | 31:RH:79:VAL:HG22  | 2.14                     | 0.47              |
| 25:YA:345:A:O2'   | 25:YA:346:A:N7     | 2.43                     | 0.47              |
| 27:RD:260:ARG:NH1 | 27:RD:267:SER:OG   | 2.48                     | 0.47              |
| 35:RP:59:LEU:CD1  | 54:R8:56:GLU:HG3   | 2.32                     | 0.47              |
| 22:QV:2:G:O2'     | 22:QV:3:C:O5'      | 2.30                     | 0.47              |
| 25:YA:141:A:C8    | 25:YA:1408:C:H1'   | 2.50                     | 0.47              |
| 34:YO:98:VAL:HG22 | 34:YO:118:ALA:HA   | 1.96                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 9:XI:28:VAL:HG11    | 9:XI:63:ILE:H       | 1.79                     | 0.47              |
| 52:Y6:9:LEU:HD22    | 52:Y6:10:LEU:H      | 1.80                     | 0.47              |
| 50:Y4:39:CYS:O      | 50:Y4:40:HIS:ND1    | 2.48                     | 0.47              |
| 28:YE:111:ARG:HA    | 37:YR:2:ARG:HH12    | 1.79                     | 0.47              |
| 25:RA:1794:U:H1'    | 25:RA:1900:A:N3     | 2.30                     | 0.47              |
| 1:QA:258:G:H2'      | 1:QA:259:G:C8       | 2.49                     | 0.47              |
| 5:XE:80:ILE:HD11    | 5:XE:138:ALA:HB1    | 1.97                     | 0.47              |
| 1:XA:142:G:H2'      | 1:XA:143:A:C8       | 2.50                     | 0.47              |
| 1:XA:1219:U:OP1     | 14:XN:19:ARG:NH1    | 2.46                     | 0.47              |
| 25:YA:1168:G:H2'    | 25:YA:1169:G:C8     | 2.50                     | 0.47              |
| 32:YI:69:LYS:HG2    | 32:YI:136:VAL:HB    | 1.97                     | 0.47              |
| 25:RA:1790:C:H5''   | 25:RA:1791:A:OP1    | 2.14                     | 0.47              |
| 25:RA:271(L):U:H5'' | 25:RA:271(M):G:C2   | 2.50                     | 0.47              |
| 17:QQ:59:ILE:HG23   | 17:QQ:71:PHE:HB3    | 1.97                     | 0.47              |
| 25:YA:1711:C:H2'    | 25:YA:1712:C:C6     | 2.50                     | 0.47              |
| 1:QA:657:G:H4'      | 15:QO:28:GLN:HG2    | 1.97                     | 0.47              |
| 1:QA:648:A:H2'      | 1:QA:649:G:H8       | 1.79                     | 0.47              |
| 17:XQ:41:LYS:HB2    | 17:XQ:41:LYS:HE3    | 1.66                     | 0.47              |
| 1:XA:1191:A:C5'     | 3:XC:4:LYS:CE       | 2.87                     | 0.47              |
| 45:RZ:126:VAL:HB    | 45:RZ:161:VAL:HG13  | 1.97                     | 0.47              |
| 25:YA:1225:C:O3'    | 41:YV:85:LYS:HD3    | 2.15                     | 0.47              |
| 40:RU:95:LEU:HD13   | 41:RV:4:ILE:HG13    | 1.96                     | 0.47              |
| 25:RA:252:G:P       | 35:RP:50:ARG:NH2    | 2.88                     | 0.47              |
| 10:QJ:50:ILE:HA     | 10:QJ:60:ARG:HB3    | 1.97                     | 0.47              |
| 5:QE:11:ILE:HG21    | 5:QE:105:VAL:HG22   | 1.97                     | 0.47              |
| 25:YA:2732:G:H3'    | 25:YA:2733:A:O4'    | 2.15                     | 0.47              |
| 35:YP:15:ARG:O      | 35:YP:17:LYS:N      | 2.48                     | 0.47              |
| 25:RA:1930:G:O2'    | 25:RA:1931:U:OP2    | 2.30                     | 0.47              |
| 48:R2:47:ASN:HB2    | 48:R2:48:HIS:H      | 1.56                     | 0.47              |
| 1:QA:559:A:H4'      | 1:QA:560:U:H5''     | 1.96                     | 0.47              |
| 25:YA:471:A:H2'     | 25:YA:472:A:O4'     | 2.14                     | 0.47              |
| 50:Y4:23:GLU:O      | 50:Y4:25:TYR:N      | 2.47                     | 0.47              |
| 18:XR:22:VAL:HG22   | 18:XR:23:LYS:H      | 1.80                     | 0.47              |
| 25:YA:270(N):G:O2'  | 25:YA:270(P):C:H5'' | 2.13                     | 0.47              |
| 49:R3:40:THR:OG1    | 49:R3:43:ILE:HG12   | 2.15                     | 0.47              |
| 14:XN:23:ARG:HD2    | 14:XN:28:GLY:O      | 2.14                     | 0.47              |
| 35:RP:65:ARG:HH22   | 54:R8:23:VAL:HG12   | 1.79                     | 0.47              |
| 1:XA:881:G:P        | 12:XL:12:ARG:HH22   | 2.37                     | 0.47              |
| 9:QI:37:PHE:CE2     | 9:QI:70:LYS:HG3     | 2.50                     | 0.47              |
| 1:XA:618:C:H5'      | 1:XA:619:U:H5''     | 1.97                     | 0.47              |
| 25:RA:1523:U:H2'    | 25:RA:1524:G:C8     | 2.50                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:YA:1424:G:H2'  | 25:YA:1425:G:O4'   | 2.14                     | 0.47              |
| 40:YU:81:HIS:HD2  | 40:YU:84:LYS:HD3   | 1.79                     | 0.47              |
| 25:RA:627:A:H4'   | 25:RA:628:G:H5'    | 1.96                     | 0.47              |
| 42:YW:94:ASP:N    | 42:YW:94:ASP:OD1   | 2.47                     | 0.47              |
| 48:Y2:5:GLU:CD    | 48:Y2:5:GLU:H      | 2.18                     | 0.47              |
| 25:YA:1465:G:H5'  | 25:YA:1528:A:O2'   | 2.15                     | 0.47              |
| 25:YA:1357:U:H2'  | 25:YA:1358:G:O4'   | 2.15                     | 0.47              |
| 37:RR:55:ALA:HB2  | 37:RR:79:LEU:HD13  | 1.96                     | 0.47              |
| 1:QA:201:C:O2'    | 1:QA:202:U:OP1     | 2.30                     | 0.47              |
| 25:YA:2850:A:N7   | 25:YA:2868:A:O2'   | 2.45                     | 0.47              |
| 28:RE:78:LEU:CD2  | 28:RE:79:ARG:CD    | 2.83                     | 0.47              |
| 31:YH:9:ILE:CB    | 31:YH:10:PRO:HA    | 2.44                     | 0.47              |
| 27:YD:35:LYS:HD3  | 27:YD:63:ARG:HG3   | 1.97                     | 0.47              |
| 9:XI:28:VAL:HG22  | 9:XI:29:ASN:H      | 1.78                     | 0.47              |
| 1:QA:1442(A):G:N7 | 39:RT:118:ARG:HB3  | 2.30                     | 0.47              |
| 19:XS:45:VAL:O    | 19:XS:47:HIS:N     | 2.44                     | 0.47              |
| 27:RD:44:ASN:HB2  | 27:RD:48:ARG:O     | 2.15                     | 0.47              |
| 25:RA:1722:A:N7   | 25:RA:1740:G:N1    | 2.62                     | 0.47              |
| 25:RA:38:A:H2'    | 25:RA:39:C:C6      | 2.50                     | 0.47              |
| 34:RO:76:ALA:HB3  | 39:RT:75:ILE:HB    | 1.96                     | 0.47              |
| 1:QA:224:C:H2'    | 1:QA:225:C:C6      | 2.50                     | 0.47              |
| 17:QQ:40:LYS:HD3  | 17:QQ:42:TYR:CZ    | 2.50                     | 0.47              |
| 25:RA:2827:C:H5'  | 25:RA:2828:C:OP2   | 2.15                     | 0.47              |
| 20:QT:29:LYS:O    | 20:QT:33:ILE:HG12  | 2.15                     | 0.47              |
| 1:QA:60:A:H4'     | 1:QA:61:G:O5'      | 2.15                     | 0.47              |
| 17:XQ:21:VAL:HG21 | 17:XQ:59:ILE:HD11  | 1.97                     | 0.47              |
| 25:YA:1916:A:H5'  | 25:YA:1917:U:OP2   | 2.14                     | 0.47              |
| 32:YI:9:LEU:HD11  | 32:YI:12:LEU:HD22  | 1.97                     | 0.47              |
| 9:XI:43:ALA:HA    | 9:XI:74:ILE:HD13   | 1.97                     | 0.47              |
| 44:RY:76:CYS:SG   | 44:RY:77:PRO:HD3   | 2.44                     | 0.46              |
| 28:RE:79:ARG:NH1  | 28:RE:164:ARG:NH1  | 2.63                     | 0.46              |
| 1:QA:1491:G:N2    | 25:RA:1913:A:N6    | 2.60                     | 0.46              |
| 38:YS:71:ARG:NH1  | 38:YS:106:ARG:HH21 | 2.13                     | 0.46              |
| 1:XA:1305:G:H5'   | 21:XU:4:GLY:HA3    | 1.96                     | 0.46              |
| 25:RA:2439:A:P    | 25:RA:2439:A:H3'   | 2.55                     | 0.46              |
| 47:R1:70:VAL:O    | 47:R1:74:VAL:HG23  | 2.15                     | 0.46              |
| 1:QA:1005:A:H3'   | 1:QA:1006:C:O4'    | 2.14                     | 0.46              |
| 19:XS:19:VAL:HG22 | 19:XS:44:MET:SD    | 2.55                     | 0.46              |
| 9:XI:2:GLU:HG3    | 9:XI:3:GLN:H       | 1.79                     | 0.46              |
| 13:QM:23:TYR:CG   | 13:QM:71:ARG:HD2   | 2.50                     | 0.46              |
| 28:YE:11:MET:HA   | 28:YE:24:THR:HA    | 1.96                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:YA:2584:U:O4'   | 25:YA:2584:U:O2   | 2.30                     | 0.46              |
| 25:YA:817:C:H4'    | 25:YA:932:G:C6    | 2.51                     | 0.46              |
| 25:YA:2115:G:OP1   | 25:YA:2167:U:N3   | 2.32                     | 0.46              |
| 22:QW:37:A:H2'     | 22:QW:38:A:O4'    | 2.15                     | 0.46              |
| 1:XA:779:C:H2'     | 1:XA:780:A:O4'    | 2.15                     | 0.46              |
| 1:XA:703:G:H4'     | 1:XA:704:A:O5'    | 2.15                     | 0.46              |
| 25:YA:1779:U:OP2   | 25:YA:1784:A:N6   | 2.45                     | 0.46              |
| 26:YB:116:G:H4'    | 38:YS:54:LEU:HD13 | 1.97                     | 0.46              |
| 25:RA:978:G:C2     | 25:RA:986:C:C2    | 3.03                     | 0.46              |
| 29:RF:192:LEU:HD23 | 29:RF:193:VAL:N   | 2.29                     | 0.46              |
| 8:XH:20:TYR:HE2    | 8:XH:75:ARG:HD2   | 1.80                     | 0.46              |
| 1:QA:1356:G:H2'    | 1:QA:1357:A:C8    | 2.50                     | 0.46              |
| 1:QA:1053:G:N7     | 1:QA:1200:C:H5''  | 2.29                     | 0.46              |
| 7:XG:104:LEU:HA    | 7:XG:104:LEU:HD13 | 1.81                     | 0.46              |
| 25:YA:2396:G:H4'   | 47:Y1:30:VAL:H    | 1.80                     | 0.46              |
| 25:RA:2593:U:H2'   | 25:RA:2594:C:C6   | 2.50                     | 0.46              |
| 45:YZ:111:VAL:O    | 45:YZ:113:ALA:N   | 2.42                     | 0.46              |
| 25:YA:2865:U:H5''  | 25:YA:2866:U:H2'  | 1.96                     | 0.46              |
| 1:XA:1379:G:O6     | 7:XG:3:ARG:HD2    | 2.15                     | 0.46              |
| 27:YD:43:ARG:NH1   | 27:YD:44:ASN:HD21 | 2.13                     | 0.46              |
| 52:Y6:27:LYS:HE2   | 52:Y6:27:LYS:HB2  | 1.23                     | 0.46              |
| 1:QA:543:C:OP1     | 4:QD:14:ARG:NE    | 2.49                     | 0.46              |
| 25:YA:2646:C:N4    | 25:YA:2732:G:N1   | 2.64                     | 0.46              |
| 39:RT:95:ARG:O     | 39:RT:96:ARG:HB2  | 2.16                     | 0.46              |
| 35:RP:23:PRO:C     | 35:RP:25:SER:H    | 2.19                     | 0.46              |
| 25:YA:2267:A:H5''  | 25:YA:2268:A:H5'  | 1.97                     | 0.46              |
| 4:QD:195:ALA:HB2   | 6:XF:20:ALA:HB2   | 1.98                     | 0.46              |
| 39:YT:74:ARG:HD3   | 39:YT:76:PHE:CE2  | 2.50                     | 0.46              |
| 35:RP:65:ARG:HE    | 54:R8:15:LYS:HB2  | 1.80                     | 0.46              |
| 11:QK:34:ASP:HB3   | 11:QK:40:ILE:HD11 | 1.96                     | 0.46              |
| 1:XA:1057:G:H2'    | 1:XA:1058:G:O4'   | 2.14                     | 0.46              |
| 25:RA:626:U:O4     | 35:RP:107:LYS:HD3 | 2.16                     | 0.46              |
| 1:QA:473:G:OP2     | 16:QP:75:ARG:NH1  | 2.48                     | 0.46              |
| 29:YF:23:ASP:OD2   | 29:YF:203:GLN:NE2 | 2.47                     | 0.46              |
| 25:RA:18:C:O2'     | 25:RA:554:U:OP1   | 2.30                     | 0.46              |
| 25:RA:1476:C:H2'   | 25:RA:1477:A:C8   | 2.50                     | 0.46              |
| 36:YQ:35:VAL:CG1   | 36:YQ:130:LYS:HB3 | 2.45                     | 0.46              |
| 26:RB:44:G:O2'     | 26:RB:47:C:N4     | 2.48                     | 0.46              |
| 42:RW:13:SER:HB3   | 42:RW:16:LYS:HD2  | 1.98                     | 0.46              |
| 44:RY:81:LYS:HD3   | 44:RY:97:ARG:CZ   | 2.45                     | 0.46              |
| 28:RE:35:GLN:HG3   | 28:RE:64:LYS:NZ   | 2.30                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:1224:C:C4'  | 41:RV:85:LYS:HB2   | 2.29                     | 0.46              |
| 25:YA:6:A:C2      | 25:YA:7:G:C8       | 3.03                     | 0.46              |
| 25:RA:848:G:O6    | 25:RA:928:G:H2'    | 2.15                     | 0.46              |
| 1:XA:316:G:P      | 1:XA:351:G:O2'     | 2.74                     | 0.46              |
| 43:RX:63:LYS:H    | 43:RX:63:LYS:CE    | 2.28                     | 0.46              |
| 25:RA:1312:U:OP2  | 43:RX:63:LYS:HD3   | 2.15                     | 0.46              |
| 10:QJ:40:LEU:HB3  | 10:QJ:69:ASN:HB2   | 1.98                     | 0.46              |
| 25:YA:2855:C:H2'  | 25:YA:2856:C:H6    | 1.80                     | 0.46              |
| 1:XA:1074:G:O2'   | 1:XA:1101:A:N1     | 2.34                     | 0.46              |
| 32:YI:7:GLU:HG3   | 32:YI:8:PRO:HD2    | 1.96                     | 0.46              |
| 25:YA:606:U:H4'   | 25:YA:658:C:H4'    | 1.96                     | 0.46              |
| 25:RA:2577:A:H5'' | 25:RA:2578:G:H5'   | 1.97                     | 0.46              |
| 25:YA:1206:G:C6   | 25:YA:1207:C:C4    | 3.04                     | 0.46              |
| 30:RG:142:PRO:HB2 | 50:R4:31:ILE:HD12  | 1.96                     | 0.46              |
| 25:YA:861:A:N3    | 26:YB:79:C:O2'     | 2.44                     | 0.46              |
| 47:R1:94:LEU:H    | 47:R1:94:LEU:HD23  | 1.80                     | 0.46              |
| 1:XA:865:A:H2     | 1:XA:918:A:H4'     | 1.80                     | 0.46              |
| 18:QR:32:ARG:HA   | 18:QR:69:THR:HG21  | 1.97                     | 0.46              |
| 3:QC:32:LEU:O     | 3:QC:36:ASP:HB2    | 2.15                     | 0.46              |
| 25:YA:826:U:H2'   | 25:YA:828:U:O4'    | 2.15                     | 0.46              |
| 41:YV:35:LEU:HB2  | 41:YV:37:VAL:HG13  | 1.96                     | 0.46              |
| 1:XA:953:G:H2'    | 1:XA:954:G:O4'     | 2.15                     | 0.46              |
| 40:RU:92:ARG:HH22 | 41:RV:11:GLN:N     | 2.14                     | 0.46              |
| 27:YD:43:ARG:HD2  | 27:YD:44:ASN:OD1   | 2.15                     | 0.46              |
| 1:QA:716:A:N6     | 1:QA:717:C:N4      | 2.64                     | 0.46              |
| 3:QC:157:ILE:HD12 | 3:QC:164:ARG:HB3   | 1.97                     | 0.46              |
| 25:YA:299:A:N1    | 25:YA:322:A:O2'    | 2.36                     | 0.46              |
| 4:XD:18:LYS:HE2   | 4:XD:20:TYR:CE2    | 2.51                     | 0.46              |
| 19:XS:44:MET:HG2  | 19:XS:47:HIS:CE1   | 2.50                     | 0.46              |
| 28:YE:134:ILE:C   | 28:YE:134:ILE:HD13 | 2.36                     | 0.46              |
| 29:RF:122:LYS:HD2 | 29:RF:191:ARG:HG2  | 1.97                     | 0.46              |
| 25:YA:248:G:H5'   | 25:YA:250:G:N7     | 2.31                     | 0.46              |
| 20:QT:26:ASN:HB2  | 20:QT:71:THR:HG23  | 1.98                     | 0.46              |
| 1:XA:21:G:H2'     | 1:XA:22:G:C8       | 2.50                     | 0.46              |
| 25:YA:848:G:H2'   | 25:YA:849:A:C8     | 2.50                     | 0.46              |
| 28:YE:14:ILE:HD11 | 28:YE:173:VAL:HG11 | 1.97                     | 0.46              |
| 25:RA:2811:G:N2   | 25:RA:2891:G:H1'   | 2.31                     | 0.46              |
| 34:RO:120:GLU:OE1 | 39:RT:67:SER:OG    | 2.32                     | 0.46              |
| 22:QW:8:U:O4'     | 22:QW:48:C:O2'     | 2.33                     | 0.46              |
| 25:YA:1125:G:C6   | 25:YA:1126:A:N6    | 2.83                     | 0.46              |
| 25:RA:994:C:OP1   | 40:RU:53:ARG:NH2   | 2.48                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:XF:61:LEU:HB3    | 6:XF:63:TYR:HE2    | 1.79                     | 0.46              |
| 44:RY:4:LYS:HA     | 44:RY:4:LYS:HE2    | 1.96                     | 0.46              |
| 25:RA:570:G:H2'    | 25:RA:2030:A:C5    | 2.49                     | 0.46              |
| 1:QA:41:G:H2'      | 1:QA:42:G:C8       | 2.49                     | 0.46              |
| 25:YA:2749:A:H4'   | 31:YH:62:LYS:HD3   | 1.97                     | 0.46              |
| 25:RA:2446:G:O2'   | 25:RA:2448:A:H5''  | 2.15                     | 0.46              |
| 52:Y6:28:ARG:HG3   | 52:Y6:30:THR:C     | 2.35                     | 0.46              |
| 1:XA:1001(A):G:OP1 | 1:XA:1001(A):G:H4' | 2.14                     | 0.46              |
| 30:YG:83:ARG:N     | 30:YG:86:MET:HG3   | 2.30                     | 0.46              |
| 25:YA:1301:A:O2'   | 25:YA:1302:A:H3'   | 2.15                     | 0.46              |
| 25:RA:779:U:OP1    | 27:RD:49:ILE:HG23  | 2.16                     | 0.46              |
| 25:YA:252:G:OP2    | 35:YP:50:ARG:NH2   | 2.48                     | 0.46              |
| 1:XA:946:A:H2'     | 1:XA:947:G:C8      | 2.50                     | 0.46              |
| 1:XA:908:A:H2'     | 1:XA:909:A:C8      | 2.50                     | 0.46              |
| 35:RP:65:ARG:O     | 35:RP:68:GLN:NE2   | 2.41                     | 0.46              |
| 40:YU:24:TYR:HB2   | 40:YU:29:SER:HB3   | 1.97                     | 0.46              |
| 1:XA:858:G:O6      | 1:XA:869:G:H3'     | 2.15                     | 0.46              |
| 22:XW:23:C:H2'     | 22:XW:24:U:C6      | 2.50                     | 0.46              |
| 25:YA:708:C:H42    | 25:YA:723:G:H1     | 1.62                     | 0.46              |
| 25:YA:754:C:H2'    | 25:YA:755:C:C6     | 2.50                     | 0.46              |
| 1:XA:977:A:O2'     | 1:XA:981:U:N3      | 2.46                     | 0.46              |
| 1:QA:1256:A:OP2    | 3:QC:26:LYS:NZ     | 2.37                     | 0.46              |
| 1:XA:1426:C:H2'    | 1:XA:1427:U:C6     | 2.51                     | 0.46              |
| 25:RA:1518:U:H2'   | 25:RA:1519:G:O4'   | 2.16                     | 0.46              |
| 25:YA:1053:C:H42   | 25:YA:1106:G:H1    | 1.62                     | 0.46              |
| 34:RO:8:LEU:HB2    | 34:RO:19:ILE:HG13  | 1.96                     | 0.46              |
| 33:YN:9:VAL:HG11   | 33:YN:39:ARG:HH22  | 1.80                     | 0.46              |
| 25:YA:196:A:O2'    | 25:YA:805:G:O6     | 2.22                     | 0.46              |
| 13:QM:93:ARG:HA    | 13:QM:93:ARG:HD3   | 1.53                     | 0.46              |
| 35:YP:46:LYS:HG2   | 35:YP:51:PHE:CG    | 2.50                     | 0.46              |
| 46:Y0:12:ASN:HA    | 46:Y0:14:ARG:HH21  | 1.79                     | 0.46              |
| 26:RB:15:A:H5'     | 26:RB:16:G:C8      | 2.51                     | 0.46              |
| 28:RE:35:GLN:HB2   | 28:RE:48:GLN:HB2   | 1.97                     | 0.46              |
| 7:QG:86:GLN:HE22   | 22:QW:31:G:H21     | 1.57                     | 0.46              |
| 35:RP:9:ASN:O      | 35:RP:10:PRO:C     | 2.54                     | 0.46              |
| 25:RA:1342:A:H2    | 25:RA:1602:U:N3    | 2.04                     | 0.46              |
| 22:QW:18:G:H4'     | 22:QW:60:U:C2      | 2.50                     | 0.46              |
| 19:QS:5:LEU:HD12   | 19:QS:5:LEU:H      | 1.80                     | 0.46              |
| 12:QL:47:LYS:HB3   | 12:QL:48:PRO:CD    | 2.44                     | 0.46              |
| 53:Y7:5:TRP:NE1    | 53:Y7:7:PRO:HG3    | 2.31                     | 0.46              |
| 25:RA:1754:C:H2'   | 25:RA:1755:A:C8    | 2.51                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:QB:194:PRO:O    | 2:QB:197:VAL:N     | 2.48                     | 0.46              |
| 25:YA:674:G:O2'   | 29:YF:74:ARG:HG3   | 2.16                     | 0.46              |
| 25:RA:2022:U:O2'  | 25:RA:2617:C:H5'   | 2.15                     | 0.46              |
| 41:RV:30:GLY:H    | 41:RV:61:VAL:CG1   | 2.29                     | 0.46              |
| 1:XA:1256:A:OP2   | 3:XC:26:LYS:NZ     | 2.39                     | 0.46              |
| 1:QA:1237:C:H2'   | 1:QA:1238:A:OP1    | 2.16                     | 0.46              |
| 27:RD:77:ALA:HB2  | 27:RD:97:TYR:CD2   | 2.50                     | 0.46              |
| 1:QA:518:C:H2'    | 1:QA:530:G:C8      | 2.50                     | 0.46              |
| 26:RB:89:G:H2'    | 26:RB:89(A):A:C8   | 2.50                     | 0.46              |
| 1:XA:620:C:H2'    | 1:XA:621:A:O4'     | 2.15                     | 0.46              |
| 1:XA:598:U:H2'    | 1:XA:599:C:C6      | 2.51                     | 0.46              |
| 25:RA:492:A:H2'   | 25:RA:493:G:O4'    | 2.14                     | 0.46              |
| 25:YA:1935:G:H1'  | 25:YA:1964:G:N2    | 2.31                     | 0.46              |
| 1:QA:160:A:H2'    | 1:QA:161:A:O4'     | 2.14                     | 0.46              |
| 30:YG:171:ALA:O   | 30:YG:175:LEU:HG   | 2.15                     | 0.46              |
| 25:RA:1991:U:H2'  | 25:RA:1992:G:H5''  | 1.98                     | 0.46              |
| 35:YP:57:THR:HG23 | 35:YP:60:MET:HB2   | 1.97                     | 0.46              |
| 19:QS:36:ARG:NH1  | 19:QS:73:GLU:H     | 2.14                     | 0.46              |
| 40:RU:92:ARG:HH22 | 41:RV:10:LYS:HA    | 1.79                     | 0.46              |
| 25:RA:1024:G:H8   | 25:RA:1024:G:O5'   | 1.98                     | 0.46              |
| 1:QA:675:A:H1'    | 11:QK:116:HIS:NE2  | 2.31                     | 0.46              |
| 28:YE:134:ILE:N   | 28:YE:134:ILE:CD1  | 2.78                     | 0.46              |
| 17:XQ:58:GLU:O    | 17:XQ:74:LEU:N     | 2.46                     | 0.46              |
| 1:QA:313:A:H2'    | 1:QA:314:C:C6      | 2.51                     | 0.46              |
| 2:QB:91:PRO:HA    | 2:QB:154:LEU:HD11  | 1.97                     | 0.46              |
| 1:XA:1515:C:H2'   | 1:XA:1516:G:C8     | 2.50                     | 0.46              |
| 42:YW:58:ALA:HB1  | 42:YW:64:MET:HB2   | 1.98                     | 0.46              |
| 1:QA:216:G:H2'    | 1:QA:217:C:C6      | 2.51                     | 0.46              |
| 22:XW:9:G:N7      | 22:XW:23:C:N4      | 2.63                     | 0.46              |
| 1:XA:412:A:C6     | 4:XD:35:ARG:HG2    | 2.51                     | 0.46              |
| 25:RA:580:C:H2'   | 25:RA:581:C:C6     | 2.51                     | 0.46              |
| 25:YA:1012:U:O4   | 33:YN:25:ARG:HA    | 2.15                     | 0.46              |
| 25:YA:675:A:OP1   | 29:YF:63:LYS:NZ    | 2.37                     | 0.46              |
| 25:YA:121:G:H4'   | 25:YA:149:A:H5'    | 1.97                     | 0.46              |
| 1:XA:160:A:H2'    | 1:XA:161:A:O4'     | 2.16                     | 0.46              |
| 31:RH:38:SER:O    | 31:RH:40:GLU:N     | 2.49                     | 0.46              |
| 1:QA:31:G:O2'     | 1:QA:48:C:N4       | 2.48                     | 0.46              |
| 25:YA:117:G:H4'   | 53:Y7:18:PHE:CE2   | 2.50                     | 0.46              |
| 35:RP:98:GLU:HA   | 35:RP:101:VAL:HG12 | 1.98                     | 0.46              |
| 25:YA:289:A:H5'   | 25:YA:290:G:OP2    | 2.16                     | 0.46              |
| 54:R8:16:ILE:HD11 | 54:R8:60:LEU:HD12  | 1.98                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:1060:C:H3'    | 3:XC:3:ASN:HD21   | 1.80                     | 0.46              |
| 25:RA:1301:A:HO2'  | 25:RA:1302:A:H3'  | 1.74                     | 0.46              |
| 25:RA:857:C:H1'    | 46:R0:26:TYR:CE2  | 2.49                     | 0.46              |
| 31:YH:7:LEU:HD13   | 31:YH:69:ARG:CB   | 2.46                     | 0.46              |
| 50:R4:58:ARG:O     | 50:R4:62:ARG:N    | 2.49                     | 0.46              |
| 27:YD:27:THR:O     | 27:YD:28:GLU:HB2  | 2.15                     | 0.46              |
| 38:RS:26:LEU:HD22  | 38:RS:87:PHE:HD1  | 1.81                     | 0.46              |
| 34:YO:88:ASN:OD1   | 34:YO:92:GLU:N    | 2.49                     | 0.46              |
| 26:RB:30:C:H1'     | 26:RB:57:A:H61    | 1.81                     | 0.46              |
| 22:QW:9:G:N2       | 22:QW:45:G:N7     | 2.64                     | 0.46              |
| 25:RA:639:U:H2'    | 25:RA:640:C:C6    | 2.51                     | 0.46              |
| 25:YA:443:A:N7     | 29:YF:45:ARG:HG3  | 2.31                     | 0.46              |
| 32:RI:76:THR:H     | 32:RI:77:LEU:HD23 | 1.81                     | 0.46              |
| 38:YS:29:PHE:HB3   | 38:YS:36:TYR:HB2  | 1.98                     | 0.46              |
| 13:XM:73:GLU:OE1   | 13:XM:77:ASN:ND2  | 2.48                     | 0.46              |
| 25:RA:1268:A:C2    | 25:RA:1269:A:H1'  | 2.51                     | 0.46              |
| 32:YI:12:LEU:HG    | 32:YI:19:VAL:HG11 | 1.97                     | 0.46              |
| 34:RO:2:ILE:HG21   | 34:RO:8:LEU:HD21  | 1.98                     | 0.46              |
| 25:YA:99:U:O2      | 25:YA:102:G:N1    | 2.49                     | 0.46              |
| 25:RA:623:G:H2'    | 25:RA:624:C:C6    | 2.51                     | 0.46              |
| 4:QD:22:LYS:O      | 4:QD:113:SER:HB2  | 2.16                     | 0.46              |
| 25:YA:363(B):G:H2' | 25:YA:363(C):G:H8 | 1.80                     | 0.46              |
| 22:QW:26:G:H1      | 22:QW:44:A:H61    | 1.64                     | 0.46              |
| 1:XA:54:C:N4       | 1:XA:353:A:OP2    | 2.43                     | 0.46              |
| 19:XS:38:SER:HB2   | 19:XS:39:THR:H    | 1.63                     | 0.46              |
| 11:QK:116:HIS:O    | 11:QK:117:ASN:HB2 | 2.15                     | 0.46              |
| 52:R6:9:LEU:N      | 52:R6:27:LYS:HA   | 2.29                     | 0.46              |
| 1:QA:354:G:C6      | 1:QA:355:C:N4     | 2.84                     | 0.46              |
| 10:XJ:45:ARG:HB3   | 10:XJ:65:LEU:HB3  | 1.98                     | 0.46              |
| 1:XA:757:U:OP1     | 1:XA:822:C:O2'    | 2.28                     | 0.46              |
| 25:RA:644:A:H4'    | 25:RA:645:C:C5    | 2.51                     | 0.46              |
| 1:XA:359:U:H2'     | 1:XA:360:A:H8     | 1.80                     | 0.46              |
| 25:RA:2557:G:H2'   | 25:RA:2558:C:C6   | 2.51                     | 0.46              |
| 28:RE:144:ARG:HB3  | 28:RE:145:LYS:H   | 1.44                     | 0.46              |
| 51:Y5:51:TYR:HB3   | 51:Y5:52:TYR:H    | 1.51                     | 0.46              |
| 17:XQ:59:ILE:HG22  | 17:XQ:71:PHE:CD1  | 2.51                     | 0.46              |
| 42:RW:13:SER:HA    | 42:RW:14:PRO:HD3  | 1.83                     | 0.46              |
| 25:YA:1075:C:H2'   | 25:YA:1076:C:C6   | 2.51                     | 0.46              |
| 38:YS:59:LYS:HD3   | 38:YS:60:GLY:H    | 1.81                     | 0.46              |
| 13:XM:14:ARG:HA    | 13:XM:43:THR:O    | 2.16                     | 0.46              |
| 25:YA:2516:G:C6    | 25:YA:2517:C:C4   | 3.04                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:QY:33:ARG:O    | 24:QY:37:ILE:HG13  | 2.16                     | 0.46              |
| 19:QS:33:THR:OG1  | 19:QS:34:TRP:N     | 2.48                     | 0.46              |
| 25:RA:443:A:H5''  | 25:RA:444:C:OP1    | 2.16                     | 0.46              |
| 47:Y1:92:LYS:HE2  | 47:Y1:92:LYS:HB3   | 1.78                     | 0.46              |
| 25:YA:2757:A:OP1  | 55:Y9:19:ARG:HA    | 2.16                     | 0.46              |
| 25:RA:1809:A:H2'  | 25:RA:1810:A:C8    | 2.51                     | 0.46              |
| 44:RY:96:ILE:HD12 | 44:RY:98:VAL:HG12  | 1.96                     | 0.46              |
| 35:YP:62:LEU:O    | 54:Y8:13:ARG:HG2   | 2.15                     | 0.46              |
| 45:RZ:150:LEU:O   | 45:RZ:155:LEU:HD21 | 2.16                     | 0.46              |
| 22:XV:54:U:H2'    | 22:XV:55:U:C5'     | 2.46                     | 0.46              |
| 35:YP:9:ASN:O     | 35:YP:10:PRO:C     | 2.53                     | 0.46              |
| 1:XA:1235:U:O2'   | 1:XA:1305:G:O5'    | 2.34                     | 0.46              |
| 54:R8:54:GLU:O    | 54:R8:57:ARG:N     | 2.40                     | 0.46              |
| 26:YB:80:U:H2'    | 26:YB:81:G:N2      | 2.29                     | 0.46              |
| 38:YS:17:ARG:HG3  | 38:YS:17:ARG:NH1   | 2.28                     | 0.46              |
| 1:XA:410:G:H2'    | 1:XA:429:U:C4      | 2.51                     | 0.46              |
| 6:QF:4:TYR:CE1    | 6:QF:92:LYS:HG2    | 2.51                     | 0.46              |
| 35:RP:37:GLY:O    | 35:RP:41:ARG:HG2   | 2.16                     | 0.46              |
| 16:XP:71:ARG:HG3  | 16:XP:80:PHE:CE1   | 2.50                     | 0.46              |
| 3:QC:7:PRO:O      | 3:QC:11:ARG:NH1    | 2.49                     | 0.46              |
| 1:XA:413:G:N2     | 1:XA:428:G:H1'     | 2.31                     | 0.46              |
| 3:QC:62:ASP:HA    | 3:QC:97:LYS:HD2    | 1.96                     | 0.46              |
| 44:YY:46:LYS:HD3  | 44:YY:63:LYS:HB3   | 1.97                     | 0.46              |
| 25:YA:2748:A:H8   | 31:YH:63:SER:HB3   | 1.79                     | 0.46              |
| 25:RA:1814:G:C4'  | 27:RD:51:VAL:HG21  | 2.46                     | 0.46              |
| 11:XK:13:GLN:HE21 | 11:XK:76:GLY:HA3   | 1.81                     | 0.46              |
| 1:XA:865:A:C2     | 1:XA:918:A:H4'     | 2.51                     | 0.46              |
| 1:QA:757:U:O2'    | 1:QA:879:C:O2      | 2.34                     | 0.46              |
| 3:QC:71:ALA:HB1   | 3:QC:109:PRO:HG3   | 1.97                     | 0.46              |
| 25:RA:969:U:H2'   | 25:RA:970:C:C6     | 2.51                     | 0.46              |
| 25:YA:952:G:OP1   | 36:YQ:16:ARG:NH1   | 2.40                     | 0.46              |
| 1:XA:1337:G:H5''  | 1:XA:1338:G:OP1    | 2.16                     | 0.46              |
| 25:YA:2183:C:H2'  | 25:YA:2184:G:C8    | 2.51                     | 0.46              |
| 40:YU:44:ASN:HD21 | 41:YV:75:PHE:HB3   | 1.80                     | 0.46              |
| 1:QA:7:G:H5'      | 1:QA:298:A:O4'     | 2.16                     | 0.46              |
| 26:RB:14:U:H5''   | 26:RB:71:C:O4'     | 2.15                     | 0.46              |
| 9:QI:43:ALA:HA    | 9:QI:74:ILE:HD13   | 1.97                     | 0.46              |
| 31:RH:9:ILE:O     | 31:RH:69:ARG:CD    | 2.64                     | 0.45              |
| 25:YA:2394:C:OP1  | 35:YP:63:PRO:CD    | 2.63                     | 0.45              |
| 44:YY:99:CYS:SG   | 44:YY:100:ALA:N    | 2.86                     | 0.45              |
| 47:Y1:53:VAL:HB   | 47:Y1:58:ILE:HD12  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:XX:14:A:C2'    | 23:XX:15:A:H5'    | 2.46                     | 0.45              |
| 27:YD:43:ARG:NH1  | 27:YD:44:ASN:ND2  | 2.64                     | 0.45              |
| 52:Y6:8:LYS:CG    | 52:Y6:27:LYS:HG2  | 2.46                     | 0.45              |
| 25:YA:1190:G:H5'  | 35:YP:32:THR:HA   | 1.97                     | 0.45              |
| 51:Y5:2:ALA:C     | 51:Y5:3:LYS:HD2   | 2.36                     | 0.45              |
| 1:XA:501:C:H2'    | 1:XA:502:G:C8     | 2.51                     | 0.45              |
| 31:YH:86:GLU:H    | 31:YH:86:GLU:CD   | 2.19                     | 0.45              |
| 1:XA:1316:G:N2    | 1:XA:1318:A:H3'   | 2.31                     | 0.45              |
| 25:RA:2129:C:H3'  | 25:RA:2130:U:C5'  | 2.46                     | 0.45              |
| 1:QA:1497:G:O2'   | 1:QA:1498:U:H5'   | 2.17                     | 0.45              |
| 25:RA:956:G:OP2   | 36:RQ:14:ARG:NH2  | 2.46                     | 0.45              |
| 17:QQ:92:ARG:HA   | 17:QQ:95:TYR:CE2  | 2.50                     | 0.45              |
| 1:QA:1118:C:OP1   | 9:QI:104:ARG:NH1  | 2.48                     | 0.45              |
| 37:RR:78:LYS:O    | 37:RR:82:GLU:HB3  | 2.15                     | 0.45              |
| 8:XH:51:VAL:HG11  | 8:XH:60:ARG:HH11  | 1.80                     | 0.45              |
| 25:YA:394:A:C6    | 25:YA:395:U:C4    | 3.04                     | 0.45              |
| 39:YT:51:ARG:HG2  | 39:YT:98:LYS:HE2  | 1.98                     | 0.45              |
| 25:RA:888:C:H4'   | 25:RA:889:C:H5    | 1.81                     | 0.45              |
| 25:RA:1999:C:H4'  | 25:RA:2723:C:O2   | 2.15                     | 0.45              |
| 30:YG:174:GLU:HG2 | 30:YG:180:PHE:HD1 | 1.81                     | 0.45              |
| 46:Y0:80:HIS:CD2  | 46:Y0:82:ARG:HH21 | 2.34                     | 0.45              |
| 1:XA:176:C:H2'    | 1:XA:177:C:C6     | 2.51                     | 0.45              |
| 7:QG:78:ARG:HB3   | 7:QG:79:ARG:H     | 1.57                     | 0.45              |
| 45:RZ:35:ARG:HH12 | 45:RZ:61:LEU:HD22 | 1.80                     | 0.45              |
| 45:RZ:94:GLU:HG3  | 45:RZ:129:SER:OG  | 2.17                     | 0.45              |
| 25:YA:988:A:H3'   | 49:Y3:11:SER:OG   | 2.16                     | 0.45              |
| 54:R8:30:ARG:HG3  | 54:R8:31:HIS:HB2  | 1.96                     | 0.45              |
| 1:XA:352:C:H2'    | 1:XA:353:A:OP2    | 2.16                     | 0.45              |
| 29:RF:4:VAL:HG13  | 29:RF:19:GLU:CD   | 2.36                     | 0.45              |
| 2:XB:162:ILE:HD11 | 2:XB:184:VAL:HG22 | 1.97                     | 0.45              |
| 9:XI:16:ARG:O     | 9:XI:63:ILE:HA    | 2.16                     | 0.45              |
| 26:YB:14:U:H5''   | 26:YB:71:C:O4'    | 2.16                     | 0.45              |
| 12:QL:87:GLY:HA2  | 12:QL:98:TYR:HD2  | 1.80                     | 0.45              |
| 25:RA:2286:A:C8   | 25:RA:2287:A:C6   | 3.04                     | 0.45              |
| 17:QQ:69:LYS:H    | 17:QQ:70:ARG:HD2  | 1.81                     | 0.45              |
| 25:RA:380:U:H5'   | 47:R1:18:ILE:HD12 | 1.98                     | 0.45              |
| 38:RS:39:ILE:HD12 | 38:RS:85:VAL:HG11 | 1.99                     | 0.45              |
| 45:RZ:110:GLY:H   | 45:RZ:142:SER:HB2 | 1.80                     | 0.45              |
| 3:XC:161:GLU:O    | 3:XC:162:GLN:HB2  | 2.16                     | 0.45              |
| 38:YS:4:LEU:HD23  | 38:YS:8:GLU:HG3   | 1.97                     | 0.45              |
| 1:XA:686:U:O4     | 1:XA:703:G:H1'    | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:XA:176:C:H2'    | 1:XA:177:C:H6     | 1.81                     | 0.45              |
| 38:RS:61:ASN:O    | 38:RS:65:VAL:N    | 2.46                     | 0.45              |
| 25:YA:16:G:H2'    | 25:YA:17:G:H8     | 1.82                     | 0.45              |
| 25:YA:17:G:H4'    | 40:YU:25:TRP:CH2  | 2.51                     | 0.45              |
| 25:YA:586:A:N1    | 25:YA:809:G:O2'   | 2.34                     | 0.45              |
| 44:RY:28:LYS:O    | 44:RY:38:ILE:HG23 | 2.15                     | 0.45              |
| 21:QU:25:LYS:HG2  | 21:QU:26:LYS:HG2  | 1.97                     | 0.45              |
| 45:RZ:24:LEU:HD22 | 45:RZ:41:LEU:HD23 | 1.97                     | 0.45              |
| 8:QH:23:SER:HB3   | 8:QH:62:TYR:CD1   | 2.51                     | 0.45              |
| 31:YH:77:LYS:HA   | 31:YH:77:LYS:HD2  | 1.72                     | 0.45              |
| 1:XA:1468:A:H2'   | 1:XA:1469:G:O4'   | 2.17                     | 0.45              |
| 1:XA:1069:C:O2'   | 1:XA:1192:C:H1'   | 2.16                     | 0.45              |
| 25:RA:370:G:H4'   | 25:RA:371:A:OP2   | 2.16                     | 0.45              |
| 1:XA:1386:G:H2'   | 1:XA:1387:G:H8    | 1.82                     | 0.45              |
| 25:RA:2844:G:H3'  | 25:RA:2845:G:H8   | 1.81                     | 0.45              |
| 40:RU:50:ARG:HH22 | 41:RV:72:VAL:HG23 | 1.80                     | 0.45              |
| 54:Y8:60:LEU:O    | 54:Y8:63:PRO:HD2  | 2.16                     | 0.45              |
| 31:YH:50:VAL:HG22 | 31:YH:52:VAL:H    | 1.81                     | 0.45              |
| 31:YH:7:LEU:HD12  | 31:YH:65:HIS:CE1  | 2.51                     | 0.45              |
| 29:RF:2:LYS:CB    | 29:RF:24:LEU:HD12 | 2.47                     | 0.45              |
| 29:YF:25:PRO:HB2  | 29:YF:26:ALA:H    | 1.62                     | 0.45              |
| 10:QJ:61:GLU:OE2  | 14:QN:45:ARG:NH1  | 2.49                     | 0.45              |
| 52:Y6:39:TYR:HB3  | 52:Y6:41:PRO:HD2  | 1.98                     | 0.45              |
| 25:RA:49:A:H5''   | 25:RA:51:G:O4'    | 2.17                     | 0.45              |
| 25:RA:128:C:H2'   | 25:RA:129:C:H6    | 1.81                     | 0.45              |
| 7:XG:20:ASP:OD2   | 7:XG:22:LEU:N     | 2.49                     | 0.45              |
| 1:QA:760:G:N2     | 17:QQ:94:ASN:OD1  | 2.49                     | 0.45              |
| 25:RA:2286:A:H4'  | 25:RA:2287:A:O4'  | 2.17                     | 0.45              |
| 14:QN:23:ARG:HD2  | 14:QN:28:GLY:O    | 2.16                     | 0.45              |
| 2:XB:7:VAL:O      | 2:XB:217:ARG:NH2  | 2.48                     | 0.45              |
| 25:RA:2032:G:O2'  | 28:RE:145:LYS:NZ  | 2.42                     | 0.45              |
| 34:YO:75:SER:HB2  | 39:YT:74:ARG:HH12 | 1.81                     | 0.45              |
| 26:YB:114:G:H2'   | 26:YB:115:G:C8    | 2.51                     | 0.45              |
| 14:XN:6:LEU:HD23  | 14:XN:9:LYS:HD3   | 1.98                     | 0.45              |
| 25:YA:746:A:C5    | 25:YA:2611:U:H5'' | 2.51                     | 0.45              |
| 1:XA:586:C:OP1    | 17:XQ:34:LYS:NZ   | 2.44                     | 0.45              |
| 1:XA:313:A:H2'    | 1:XA:314:C:C6     | 2.51                     | 0.45              |
| 19:QS:11:VAL:HG13 | 19:QS:39:THR:H    | 1.81                     | 0.45              |
| 1:QA:540:G:H2'    | 1:QA:541:G:O4'    | 2.16                     | 0.45              |
| 25:YA:2849:U:OP1  | 39:YT:95:ARG:NH1  | 2.49                     | 0.45              |
| 45:YZ:52:SER:O    | 45:YZ:54:HIS:N    | 2.49                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:45:U:H2'     | 1:QA:46:G:C8      | 2.51                     | 0.45              |
| 41:RV:49:THR:HG22 | 41:RV:50:PRO:N    | 2.29                     | 0.45              |
| 32:YI:77:LEU:HB2  | 32:YI:141:LYS:CB  | 2.47                     | 0.45              |
| 25:RA:2447:G:O2'  | 25:RA:2500:U:OP2  | 2.25                     | 0.45              |
| 25:RA:2393:A:H2'  | 25:RA:2394:C:O4'  | 2.16                     | 0.45              |
| 25:YA:2030:A:H4'  | 25:YA:2031:A:C8   | 2.51                     | 0.45              |
| 31:RH:159:GLU:HG3 | 31:RH:170:ARG:NH1 | 2.31                     | 0.45              |
| 55:R9:1:MET:N     | 55:R9:1:MET:SD    | 2.89                     | 0.45              |
| 31:YH:94:TYR:OH   | 31:YH:153:LYS:HE2 | 2.16                     | 0.45              |
| 39:YT:104:ASN:O   | 39:YT:106:SER:N   | 2.49                     | 0.45              |
| 25:RA:185:U:H2'   | 25:RA:186:G:C8    | 2.50                     | 0.45              |
| 1:QA:1496:C:H2'   | 1:QA:1497:G:O4'   | 2.17                     | 0.45              |
| 35:RP:36:LYS:HB3  | 35:RP:37:GLY:HA2  | 1.97                     | 0.45              |
| 25:RA:749:C:O2    | 25:RA:1618:A:H2'  | 2.16                     | 0.45              |
| 28:RE:131:ALA:HB1 | 28:RE:135:HIS:CE1 | 2.51                     | 0.45              |
| 25:YA:1657:C:H2'  | 25:YA:1658:C:C6   | 2.51                     | 0.45              |
| 50:R4:26:SER:OG   | 50:R4:27:THR:N    | 2.48                     | 0.45              |
| 22:QW:6:G:H2'     | 22:QW:7:G:H8      | 1.80                     | 0.45              |
| 25:YA:1797:C:H4'  | 27:YD:257:LEU:O   | 2.16                     | 0.45              |
| 25:YA:154:G:H5'   | 25:YA:155:C:OP2   | 2.17                     | 0.45              |
| 25:RA:1762:A:H8   | 25:RA:1762:A:O5'  | 1.99                     | 0.45              |
| 43:YX:67:GLY:O    | 43:YX:69:TYR:N    | 2.42                     | 0.45              |
| 3:QC:177:THR:HG23 | 3:QC:180:ALA:HB2  | 1.98                     | 0.45              |
| 25:YA:724:U:H2'   | 25:YA:725:G:O4'   | 2.17                     | 0.45              |
| 13:XM:15:VAL:HG12 | 13:XM:45:VAL:HG22 | 1.99                     | 0.45              |
| 44:YY:84:ARG:CZ   | 44:YY:97:ARG:HB2  | 2.46                     | 0.45              |
| 45:YZ:150:LEU:CB  | 45:YZ:171:ILE:H   | 2.29                     | 0.45              |
| 25:RA:70:G:O4'    | 25:RA:73:A:H1'    | 2.17                     | 0.45              |
| 23:QX:12:A:H8     | 23:QX:13:A:C8     | 2.34                     | 0.45              |
| 1:QA:926:G:C6     | 1:QA:1505:G:C6    | 3.05                     | 0.45              |
| 25:RA:748:G:C2'   | 25:RA:750:A:OP2   | 2.60                     | 0.45              |
| 1:QA:979:C:OP1    | 1:QA:1223:C:N4    | 2.49                     | 0.45              |
| 1:XA:960:U:O2'    | 1:XA:1223:C:H4'   | 2.17                     | 0.45              |
| 41:YV:4:ILE:HB    | 41:YV:40:LEU:HB2  | 1.98                     | 0.45              |
| 25:RA:394:A:C2'   | 25:RA:395:U:H5''  | 2.44                     | 0.45              |
| 42:RW:18:ARG:HD3  | 42:RW:76:VAL:CG1  | 2.44                     | 0.45              |
| 9:XI:28:VAL:HG21  | 9:XI:63:ILE:H     | 1.81                     | 0.45              |
| 25:YA:858:U:O2    | 25:YA:2268:A:H2'  | 2.16                     | 0.45              |
| 31:RH:3:ARG:HH11  | 31:RH:6:ARG:NE    | 2.14                     | 0.45              |
| 27:RD:30:GLU:HG3  | 27:RD:63:ARG:CZ   | 2.47                     | 0.45              |
| 55:R9:1:MET:HB3   | 55:R9:4:ARG:CZ    | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:1051:C:H2'   | 1:QA:1052:U:H6    | 1.82                     | 0.45              |
| 20:XT:14:LYS:O    | 20:XT:18:GLN:HG3  | 2.16                     | 0.45              |
| 1:QA:192:U:H2'    | 1:QA:193:C:H6     | 1.82                     | 0.45              |
| 25:YA:593:G:O4'   | 54:Y8:4:MET:HE1   | 2.16                     | 0.45              |
| 28:RE:21:VAL:HA   | 28:RE:22:PRO:HD2  | 1.74                     | 0.45              |
| 25:YA:1846:G:H5'  | 25:YA:1847:A:OP2  | 2.17                     | 0.45              |
| 25:RA:1316:U:H2'  | 25:RA:1317:A:C8   | 2.52                     | 0.45              |
| 25:YA:2080:G:H5'  | 47:Y1:19:GLN:HG3  | 1.98                     | 0.45              |
| 25:RA:2645:G:H3'  | 25:RA:2646:C:C5'  | 2.46                     | 0.45              |
| 25:RA:1956:U:H1'  | 25:RA:2552:U:OP1  | 2.16                     | 0.45              |
| 25:YA:799:G:C6    | 25:YA:800:A:C6    | 3.05                     | 0.45              |
| 7:XG:5:ARG:HH21   | 7:XG:7:ALA:HA     | 1.81                     | 0.45              |
| 35:RP:6:LEU:HD13  | 35:RP:6:LEU:HA    | 1.72                     | 0.45              |
| 29:RF:33:LEU:HD12 | 29:RF:33:LEU:HA   | 1.80                     | 0.45              |
| 34:RO:64:ARG:HB2  | 34:RO:83:ALA:HB3  | 1.99                     | 0.45              |
| 32:YI:40:THR:OG1  | 32:YI:43:ASN:OD1  | 2.33                     | 0.45              |
| 25:RA:657:U:H2'   | 25:RA:658:C:C6    | 2.50                     | 0.45              |
| 9:QI:5:TYR:HB3    | 9:QI:6:GLY:H      | 1.47                     | 0.45              |
| 1:QA:585:G:C6     | 1:QA:586:C:C4     | 3.05                     | 0.45              |
| 25:YA:463:G:N2    | 25:YA:466:A:OP2   | 2.39                     | 0.45              |
| 4:XD:178:VAL:O    | 4:XD:180:GLY:N    | 2.42                     | 0.45              |
| 48:R2:25:VAL:O    | 48:R2:29:LYS:HG3  | 2.17                     | 0.45              |
| 45:YZ:110:GLY:C   | 45:YZ:112:ARG:H   | 2.20                     | 0.45              |
| 28:RE:61:ARG:N    | 28:RE:62:PRO:HD2  | 2.31                     | 0.45              |
| 45:RZ:156:LYS:C   | 45:RZ:157:LEU:HG  | 2.37                     | 0.45              |
| 25:YA:2580:U:H4'  | 28:YE:130:GLY:CA  | 2.42                     | 0.45              |
| 1:QA:345:C:HO2'   | 1:QA:346:G:P      | 2.39                     | 0.45              |
| 43:YX:49:VAL:HB   | 43:YX:83:VAL:HG23 | 1.98                     | 0.45              |
| 48:R2:15:LYS:HD3  | 48:R2:67:LYS:HZ1  | 1.81                     | 0.45              |
| 13:QM:118:ALA:HB1 | 22:QV:28:C:O3'    | 2.17                     | 0.45              |
| 25:RA:2563:U:H2'  | 25:RA:2565:A:OP2  | 2.17                     | 0.45              |
| 1:QA:876:G:H2'    | 1:QA:877:C:C6     | 2.52                     | 0.45              |
| 3:QC:180:ALA:HB1  | 3:QC:182:ILE:HG13 | 1.98                     | 0.45              |
| 32:YI:74:ASN:HB2  | 32:YI:75:LEU:H    | 1.65                     | 0.45              |
| 25:RA:814:C:H5    | 35:RP:24:GLY:O    | 1.99                     | 0.45              |
| 41:YV:38:LEU:HA   | 41:YV:38:LEU:HD23 | 1.71                     | 0.45              |
| 1:QA:814:A:H2'    | 1:QA:816:A:H5''   | 1.99                     | 0.45              |
| 33:YN:63:THR:O    | 33:YN:66:LYS:HG3  | 2.17                     | 0.45              |
| 2:QB:37:ASN:ND2   | 2:QB:37:ASN:O     | 2.49                     | 0.45              |
| 2:XB:172:ILE:H    | 2:XB:172:ILE:HD12 | 1.82                     | 0.45              |
| 1:XA:748:C:O5'    | 1:XA:748:C:H6     | 2.00                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:XA:553:A:H5''    | 12:XL:24:VAL:HG21 | 1.98                     | 0.45              |
| 32:RI:100:ALA:O    | 32:RI:102:SER:N   | 2.49                     | 0.45              |
| 25:RA:2590:A:OP2   | 27:RD:238:GLY:HA2 | 2.17                     | 0.45              |
| 36:YQ:65:PHE:O     | 36:YQ:104:PHE:HA  | 2.17                     | 0.45              |
| 25:RA:1386:C:OP2   | 25:RA:1396:U:N3   | 2.50                     | 0.45              |
| 28:RE:61:ARG:H     | 28:RE:62:PRO:HD2  | 1.81                     | 0.45              |
| 29:RF:133:ASN:HB2  | 29:RF:138:GLU:OE1 | 2.16                     | 0.45              |
| 1:QA:67:C:H2'      | 1:QA:68:G:H8      | 1.80                     | 0.45              |
| 1:XA:191:G:H1'     | 20:XT:104:LEU:O   | 2.16                     | 0.45              |
| 3:QC:59:ARG:HG2    | 3:QC:64:VAL:HG12  | 1.99                     | 0.45              |
| 25:YA:587:C:N3     | 35:YP:33:ARG:NH1  | 2.64                     | 0.45              |
| 12:QL:58:VAL:O     | 12:QL:65:GLU:HA   | 2.16                     | 0.45              |
| 5:QE:78:HIS:HA     | 8:QH:105:ARG:HG3  | 1.98                     | 0.45              |
| 1:QA:401:C:H2'     | 1:QA:402:G:H8     | 1.82                     | 0.45              |
| 5:QE:57:LYS:O      | 5:QE:61:TYR:HD2   | 1.99                     | 0.45              |
| 25:YA:957:A:N1     | 25:YA:2458:G:H4'  | 2.32                     | 0.45              |
| 25:RA:26:G:N2      | 25:RA:513:A:OP2   | 2.42                     | 0.45              |
| 6:QF:9:VAL:HB      | 6:QF:87:ARG:HB2   | 1.97                     | 0.45              |
| 25:RA:271(E):U:H2' | 25:RA:271(F):C:C6 | 2.52                     | 0.45              |
| 49:Y3:7:LYS:HG2    | 49:Y3:9:VAL:HG13  | 1.97                     | 0.45              |
| 25:RA:1901:A:OP2   | 25:RA:1901:A:H4'  | 2.16                     | 0.45              |
| 1:XA:373:A:H2'     | 1:XA:374:A:H8     | 1.82                     | 0.45              |
| 23:QX:18:G:O3'     | 23:QX:19:A2M:H8   | 2.17                     | 0.45              |
| 1:XA:482:A:H3'     | 1:XA:483:C:H6     | 1.80                     | 0.45              |
| 1:QA:957:U:H4'     | 19:QS:79:THR:OG1  | 2.17                     | 0.45              |
| 4:XD:9:CYS:O       | 4:XD:13:ARG:HG3   | 2.16                     | 0.45              |
| 25:YA:2102:U:H2'   | 25:YA:2103:C:C6   | 2.51                     | 0.45              |
| 22:QV:52:G:H2'     | 22:QV:53:G:H5'    | 1.97                     | 0.45              |
| 52:R6:41:PRO:HD2   | 52:R6:49:HIS:NE2  | 2.32                     | 0.45              |
| 27:RD:35:LYS:HD3   | 27:RD:63:ARG:HG3  | 1.99                     | 0.45              |
| 31:YH:151:ILE:O    | 31:YH:152:ARG:HG2 | 2.15                     | 0.45              |
| 35:YP:3:LEU:HA     | 35:YP:6:LEU:HD23  | 1.98                     | 0.45              |
| 25:RA:631:A:O2'    | 35:RP:67:MET:HB3  | 2.17                     | 0.45              |
| 10:XJ:3:LYS:N      | 10:XJ:74:ILE:O    | 2.50                     | 0.45              |
| 25:RA:2286:A:H8    | 25:RA:2287:A:C6   | 2.34                     | 0.45              |
| 8:QH:51:VAL:HG11   | 8:QH:60:ARG:NH1   | 2.31                     | 0.45              |
| 1:XA:689:C:OP1     | 11:XK:27:ASN:ND2  | 2.43                     | 0.45              |
| 1:XA:707:C:H2'     | 1:XA:708:C:H6     | 1.82                     | 0.45              |
| 25:YA:270(F):U:H3  | 25:YA:270(T):G:H1 | 1.63                     | 0.45              |
| 28:RE:116:VAL:HG13 | 28:RE:122:PHE:HB2 | 1.97                     | 0.45              |
| 1:QA:298:A:H2'     | 1:QA:299:G:O4'    | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1843:C:H5'   | 27:YD:253:GLN:OE1  | 2.17                     | 0.45              |
| 34:RO:1:MET:HE2    | 34:RO:1:MET:HB3    | 1.84                     | 0.45              |
| 25:YA:2540:C:O2'   | 25:YA:2740:A:N3    | 2.44                     | 0.45              |
| 3:QC:139:GLN:O     | 3:QC:143:GLU:N     | 2.49                     | 0.45              |
| 25:YA:503:A:H4'    | 25:YA:504:U:H5''   | 1.99                     | 0.45              |
| 1:XA:1432:G:OP1    | 39:YT:107:ASP:HB2  | 2.17                     | 0.45              |
| 1:QA:1278:U:H5'    | 1:QA:1279:A:O4'    | 2.17                     | 0.45              |
| 27:RD:137:PRO:O    | 27:RD:140:THR:OG1  | 2.28                     | 0.45              |
| 19:QS:32:LYS:HE2   | 19:QS:32:LYS:HB2   | 1.76                     | 0.45              |
| 1:QA:570:G:H1'     | 1:QA:820:U:C4      | 2.52                     | 0.45              |
| 25:RA:654(T):C:H2' | 25:RA:654(U):A:O4' | 2.16                     | 0.45              |
| 29:RF:136:THR:HG23 | 29:RF:170:LEU:HD11 | 1.99                     | 0.45              |
| 25:YA:909:A:H2'    | 25:YA:912:C:C5     | 2.52                     | 0.45              |
| 41:RV:46:VAL:O     | 41:RV:48:GLY:N     | 2.50                     | 0.45              |
| 41:RV:40:LEU:CD2   | 41:RV:47:VAL:HB    | 2.47                     | 0.45              |
| 32:RI:79:ILE:O     | 32:RI:142:VAL:CG2  | 2.52                     | 0.45              |
| 1:XA:255:G:C6      | 1:XA:256:U:C4      | 3.05                     | 0.45              |
| 25:YA:1113:U:H2'   | 25:YA:1114:G:C8    | 2.52                     | 0.45              |
| 25:RA:1112:G:H2'   | 25:RA:1113:U:C6    | 2.52                     | 0.45              |
| 2:QB:33:TYR:HB3    | 2:QB:41:ILE:O      | 2.16                     | 0.45              |
| 28:YE:4:ILE:HD13   | 28:YE:95:ILE:HD13  | 1.99                     | 0.45              |
| 25:YA:910:A:H2'    | 25:YA:911:A:C8     | 2.51                     | 0.45              |
| 39:YT:26:ASP:HB2   | 39:YT:91:ARG:HA    | 1.98                     | 0.45              |
| 25:RA:2876:G:O5'   | 39:RT:3:ARG:HA     | 2.17                     | 0.45              |
| 25:RA:859:G:O2'    | 25:RA:860:U:P      | 2.75                     | 0.45              |
| 7:XG:78:ARG:HB3    | 7:XG:79:ARG:H      | 1.50                     | 0.45              |
| 43:YX:26:TYR:O     | 43:YX:81:VAL:HG22  | 2.17                     | 0.45              |
| 25:YA:218:A:H2     | 25:YA:235:U:H4'    | 1.82                     | 0.45              |
| 1:XA:619:U:N3      | 4:XD:134:ASP:OD2   | 2.36                     | 0.45              |
| 32:YI:12:LEU:HD12  | 32:YI:12:LEU:HA    | 1.79                     | 0.45              |
| 25:RA:2593:U:H2'   | 25:RA:2594:C:H6    | 1.82                     | 0.45              |
| 26:RB:15:A:H1'     | 26:RB:109:G:N9     | 2.32                     | 0.45              |
| 24:QY:37:ILE:HD11  | 24:QY:66:ILE:HD11  | 1.99                     | 0.45              |
| 1:XA:1324:A:H4'    | 1:XA:1362:C:H4'    | 1.98                     | 0.45              |
| 25:YA:1015:G:H2'   | 25:YA:1016:G:H8    | 1.82                     | 0.45              |
| 25:YA:2496:C:P     | 36:YQ:81:VAL:HG13  | 2.57                     | 0.45              |
| 1:QA:1376:U:H2'    | 1:QA:1377:A:C8     | 2.51                     | 0.45              |
| 1:XA:1510:U:H2'    | 1:XA:1511:G:C8     | 2.52                     | 0.45              |
| 13:QM:77:ASN:O     | 13:QM:80:ARG:HB2   | 2.16                     | 0.45              |
| 2:XB:97:TRP:CH2    | 2:XB:173:ALA:HA    | 2.52                     | 0.45              |
| 26:RB:94:C:H2'     | 26:RB:95:U:H6      | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:QA:1171:G:H2'   | 1:QA:1172:C:C6    | 2.52                     | 0.45              |
| 8:XH:102:ARG:H    | 8:XH:102:ARG:HG3  | 1.66                     | 0.45              |
| 25:YA:1445:C:H2'  | 25:YA:1446:C:H6   | 1.81                     | 0.45              |
| 45:RZ:107:THR:OG1 | 45:RZ:108:PRO:HD3 | 2.17                     | 0.45              |
| 7:XG:65:ALA:HB1   | 7:XG:127:ALA:HB3  | 1.98                     | 0.45              |
| 17:QQ:81:ARG:HE   | 17:QQ:84:LEU:HD12 | 1.82                     | 0.45              |
| 38:RS:27:SER:HA   | 38:RS:88:ASP:HB2  | 1.99                     | 0.45              |
| 36:RQ:78:PRO:O    | 36:RQ:79:LEU:HG   | 2.17                     | 0.45              |
| 1:QA:583:A:H2'    | 1:QA:584:G:O4'    | 2.17                     | 0.45              |
| 35:RP:57:THR:HG23 | 35:RP:60:MET:CB   | 2.37                     | 0.45              |
| 40:RU:92:ARG:HH12 | 41:RV:11:GLN:H    | 1.64                     | 0.45              |
| 1:QA:716:A:H2'    | 1:QA:717:C:O5'    | 2.17                     | 0.45              |
| 5:QE:12:LEU:HD12  | 5:QE:128:PRO:HB3  | 1.99                     | 0.45              |
| 4:QD:13:ARG:HB3   | 4:QD:14:ARG:H     | 1.51                     | 0.45              |
| 13:XM:102:ARG:HD3 | 13:XM:105:THR:OG1 | 2.17                     | 0.45              |
| 25:YA:1754:C:H2'  | 25:YA:1755:A:C8   | 2.52                     | 0.45              |
| 30:YG:16:ARG:O    | 30:YG:20:ILE:HG12 | 2.17                     | 0.45              |
| 1:QA:707:C:H2'    | 1:QA:708:C:C6     | 2.52                     | 0.45              |
| 25:YA:1813:G:H1'  | 27:YD:50:THR:OG1  | 2.17                     | 0.45              |
| 25:YA:1688:U:H1'  | 25:YA:1701:A:C6   | 2.52                     | 0.45              |
| 25:RA:66:C:H2'    | 25:RA:67:U:H6     | 1.82                     | 0.45              |
| 25:RA:534:U:H5'   | 40:RU:42:ALA:HB1  | 1.99                     | 0.45              |
| 41:RV:7:THR:HG23  | 41:RV:22:VAL:HG21 | 1.99                     | 0.45              |
| 22:XW:8:U:O4'     | 22:XW:48:C:O2'    | 2.35                     | 0.45              |
| 51:Y5:36:CYS:HB3  | 51:Y5:37:LYS:H    | 1.67                     | 0.45              |
| 45:RZ:3:TYR:HB2   | 45:RZ:57:ILE:HA   | 1.99                     | 0.45              |
| 1:XA:1356:G:H2'   | 1:XA:1357:A:C8    | 2.52                     | 0.45              |
| 51:R5:3:LYS:HE3   | 51:R5:3:LYS:HA    | 1.98                     | 0.45              |
| 29:YF:127:GLU:O   | 29:YF:129:PHE:N   | 2.49                     | 0.45              |
| 25:RA:2591:C:H2'  | 25:RA:2592:G:C8   | 2.52                     | 0.45              |
| 29:YF:46:ARG:HB3  | 29:YF:48:THR:HG23 | 1.98                     | 0.45              |
| 25:YA:2111:C:N4   | 25:YA:2118:U:O2   | 2.50                     | 0.45              |
| 26:YB:29:A:OP2    | 38:YS:32:LEU:HG   | 2.17                     | 0.45              |
| 25:RA:69:C:H6     | 25:RA:73:A:O2'    | 1.99                     | 0.44              |
| 19:QS:70:LYS:HB2  | 19:QS:71:LEU:H    | 1.68                     | 0.44              |
| 25:RA:1025:G:H8   | 25:RA:1025:G:OP1  | 2.00                     | 0.44              |
| 52:R6:15:GLU:OE2  | 52:R6:44:ARG:NH1  | 2.49                     | 0.44              |
| 25:RA:1020:A:N6   | 25:RA:1141:U:O2'  | 2.50                     | 0.44              |
| 31:RH:54:ARG:NE   | 31:RH:57:ASP:OD1  | 2.50                     | 0.44              |
| 7:XG:22:LEU:HG    | 7:XG:62:PHE:HE2   | 1.81                     | 0.44              |
| 9:XI:65:VAL:HG21  | 9:XI:73:GLN:HB3   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:R4:60:GLN:HB3  | 50:R4:61:ARG:NH2  | 2.32                     | 0.44              |
| 1:QA:444:C:H2'    | 1:QA:445:G:C8     | 2.51                     | 0.44              |
| 25:YA:928:G:H3'   | 25:YA:929:G:H8    | 1.82                     | 0.44              |
| 32:RI:56:LYS:HE3  | 32:RI:57:ARG:HG3  | 1.99                     | 0.44              |
| 41:YV:61:VAL:HA   | 41:YV:94:LEU:HD22 | 1.99                     | 0.44              |
| 26:RB:94:C:H2'    | 26:RB:95:U:C6     | 2.52                     | 0.44              |
| 25:RA:2019:A:O4'  | 40:RU:34:LYS:HD2  | 2.18                     | 0.44              |
| 48:R2:50:ILE:HD12 | 48:R2:51:ARG:H    | 1.82                     | 0.44              |
| 48:R2:4:SER:HB2   | 48:R2:5:GLU:H     | 1.45                     | 0.44              |
| 41:RV:67:GLY:O    | 41:RV:88:ARG:HD2  | 2.16                     | 0.44              |
| 29:RF:128:ALA:O   | 29:RF:142:TRP:NE1 | 2.49                     | 0.44              |
| 18:XR:32:ARG:HA   | 18:XR:69:THR:HG21 | 1.98                     | 0.44              |
| 21:QU:8:THR:HG22  | 21:QU:10:ARG:H    | 1.82                     | 0.44              |
| 20:QT:92:LEU:HA   | 20:QT:92:LEU:HD13 | 1.83                     | 0.44              |
| 25:RA:2769:C:H2'  | 25:RA:2770:G:C8   | 2.52                     | 0.44              |
| 25:YA:434:U:H1'   | 25:YA:435:C:H5    | 1.81                     | 0.44              |
| 18:QR:50:ILE:HD11 | 18:QR:70:ILE:HG21 | 1.98                     | 0.44              |
| 9:QI:85:LEU:O     | 9:QI:89:ASN:HB2   | 2.16                     | 0.44              |
| 25:YA:1165:U:H2'  | 25:YA:1166:C:C6   | 2.51                     | 0.44              |
| 25:YA:987:G:O6    | 25:YA:988:A:C2    | 2.70                     | 0.44              |
| 44:RY:17:SER:HB2  | 44:RY:71:LYS:HB3  | 1.98                     | 0.44              |
| 7:QG:77:SER:HG    | 22:QW:32:C:H4'    | 1.77                     | 0.44              |
| 1:XA:1493:A:N6    | 25:YA:1913:A:N3   | 2.65                     | 0.44              |
| 1:QA:1399:C:C2    | 1:QA:1502:A:N6    | 2.86                     | 0.44              |
| 25:RA:593:G:C1'   | 54:R8:4:MET:HE1   | 2.48                     | 0.44              |
| 1:QA:1086:U:H6    | 1:QA:1086:U:O5'   | 2.00                     | 0.44              |
| 25:RA:2429:G:N7   | 35:RP:56:SER:OG   | 2.50                     | 0.44              |
| 1:XA:501:C:H2'    | 1:XA:502:G:H8     | 1.82                     | 0.44              |
| 52:Y6:40:CYS:N    | 52:Y6:41:PRO:HD2  | 2.32                     | 0.44              |
| 1:XA:316:G:C2     | 1:XA:317:G:C5     | 3.05                     | 0.44              |
| 40:RU:76:TYR:CZ   | 40:RU:80:ILE:HG13 | 2.51                     | 0.44              |
| 19:XS:6:LYS:HG2   | 19:XS:7:LYS:H     | 1.81                     | 0.44              |
| 25:RA:2740:A:H62  | 25:RA:2763:G:H2'  | 1.83                     | 0.44              |
| 1:XA:1105:A:H2'   | 1:XA:1106:G:C8    | 2.50                     | 0.44              |
| 29:YF:117:ARG:HD2 | 29:YF:190:GLU:O   | 2.16                     | 0.44              |
| 1:QA:738:C:H5''   | 6:QF:69:GLU:HB2   | 1.98                     | 0.44              |
| 14:QN:27:CYS:HB3  | 14:QN:28:GLY:H    | 1.44                     | 0.44              |
| 2:XB:80:ILE:HD13  | 2:XB:212:GLN:HA   | 1.99                     | 0.44              |
| 25:RA:2876:G:H1'  | 39:RT:3:ARG:CZ    | 2.46                     | 0.44              |
| 25:RA:374:A:C2    | 25:RA:401:A:C4    | 3.05                     | 0.44              |
| 20:QT:14:LYS:HB2  | 20:QT:17:ARG:NH2  | 2.32                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:YU:98:LEU:C    | 40:YU:100:VAL:H    | 2.19                     | 0.44              |
| 25:YA:2039:C:H2'  | 25:YA:2040:C:H6    | 1.81                     | 0.44              |
| 3:QC:119:ARG:HH22 | 3:QC:140:ARG:HG2   | 1.81                     | 0.44              |
| 1:QA:109:A:C6     | 1:QA:326:G:C6      | 3.05                     | 0.44              |
| 31:YH:144:VAL:O   | 31:YH:148:ILE:HG12 | 2.17                     | 0.44              |
| 25:RA:2082:A:H2'  | 25:RA:2083:G:O4'   | 2.16                     | 0.44              |
| 49:Y3:43:ILE:O    | 49:Y3:47:VAL:HG23  | 2.17                     | 0.44              |
| 25:RA:2824:C:H2'  | 25:RA:2825:C:O4'   | 2.17                     | 0.44              |
| 1:QA:189(D):C:H1' | 1:QA:189(H):G:N2   | 2.32                     | 0.44              |
| 11:XK:9:LYS:HE2   | 11:XK:9:LYS:HB2    | 1.75                     | 0.44              |
| 25:YA:1625:C:H2'  | 25:YA:1626:G:O4'   | 2.17                     | 0.44              |
| 44:YY:76:CYS:HB3  | 44:YY:77:PRO:HD2   | 1.92                     | 0.44              |
| 23:XX:12:A:H3'    | 23:XX:13:A:C5'     | 2.38                     | 0.44              |
| 27:YD:43:ARG:CB   | 27:YD:54:ARG:HB2   | 2.48                     | 0.44              |
| 40:YU:50:ARG:HH11 | 41:YV:72:VAL:CG1   | 2.31                     | 0.44              |
| 45:YZ:29:TYR:CE2  | 45:YZ:87:ASP:HB2   | 2.52                     | 0.44              |
| 25:RA:2208:A:H4'  | 25:RA:2218:U:H5    | 1.82                     | 0.44              |
| 47:R1:40:ARG:NH2  | 47:R1:42:GLN:HG2   | 2.32                     | 0.44              |
| 34:YO:87:ILE:HG22 | 34:YO:88:ASN:O     | 2.18                     | 0.44              |
| 8:QH:83:ILE:HB    | 8:QH:137:VAL:HG13  | 1.99                     | 0.44              |
| 25:RA:1085:A:H2'  | 25:RA:1086:A:H8    | 1.81                     | 0.44              |
| 37:RR:38:VAL:HB   | 37:RR:39:PRO:HD3   | 1.99                     | 0.44              |
| 8:XH:4:ASP:OD2    | 8:XH:89:PRO:HD3    | 2.17                     | 0.44              |
| 22:QV:13:C:O2'    | 25:RA:1924:C:H4'   | 2.17                     | 0.44              |
| 1:QA:110:C:H2'    | 1:QA:111:G:O4'     | 2.17                     | 0.44              |
| 1:XA:503:C:H2'    | 1:XA:504:C:H6      | 1.82                     | 0.44              |
| 1:XA:793:U:OP2    | 1:XA:794:A:C8      | 2.70                     | 0.44              |
| 25:RA:1767:C:H2'  | 25:RA:1768:U:C6    | 2.51                     | 0.44              |
| 22:QW:56:C:H2'    | 22:QW:57:A:H8      | 1.83                     | 0.44              |
| 25:RA:581:C:OP1   | 40:RU:33:ARG:HG3   | 2.18                     | 0.44              |
| 25:YA:2370:G:C6   | 25:YA:2371:G:C6    | 3.05                     | 0.44              |
| 32:YI:114:LEU:HA  | 32:YI:130:TYR:HB2  | 1.98                     | 0.44              |
| 26:RB:66:A:O2'    | 26:RB:67:G:O5'     | 2.35                     | 0.44              |
| 11:XK:111:ASP:OD2 | 18:XR:84:LYS:HD2   | 2.17                     | 0.44              |
| 6:QF:44:GLY:O     | 6:QF:60:PHE:N      | 2.47                     | 0.44              |
| 7:QG:26:PHE:O     | 7:QG:30:ILE:HG12   | 2.17                     | 0.44              |
| 1:QA:512:U:H2'    | 1:QA:513:C:C6      | 2.53                     | 0.44              |
| 25:YA:1861:G:H1   | 25:YA:1881:C:H42   | 1.66                     | 0.44              |
| 26:YB:78:A:C2     | 26:YB:99:A:C4      | 3.05                     | 0.44              |
| 42:YW:46:PHE:O    | 42:YW:50:VAL:HG12  | 2.17                     | 0.44              |
| 1:QA:269:C:H2'    | 1:QA:270:A:C8      | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:YH:20:ALA:O    | 31:YH:22:GLY:N    | 2.51                     | 0.44              |
| 38:RS:14:VAL:HG21 | 38:RS:89:ARG:HD3  | 1.99                     | 0.44              |
| 9:QI:48:GLU:N     | 9:QI:49:PRO:HD2   | 2.32                     | 0.44              |
| 45:RZ:6:LYS:HB2   | 45:RZ:6:LYS:HE3   | 1.76                     | 0.44              |
| 36:YQ:103:MET:H   | 36:YQ:103:MET:HG3 | 1.53                     | 0.44              |
| 29:YF:149:ASP:OD1 | 29:YF:149:ASP:N   | 2.43                     | 0.44              |
| 25:RA:1827:C:H2'  | 25:RA:1828:G:O4'  | 2.18                     | 0.44              |
| 25:RA:197:A:N6    | 25:RA:2430:A:H2'  | 2.33                     | 0.44              |
| 25:YA:1541:U:H2'  | 25:YA:1542:G:O4'  | 2.16                     | 0.44              |
| 25:RA:1653:G:C6   | 37:RR:9:LYS:HG3   | 2.53                     | 0.44              |
| 12:QL:41:ARG:HB3  | 12:QL:42:THR:H    | 1.56                     | 0.44              |
| 28:RE:5:LEU:CD1   | 28:RE:78:LEU:O    | 2.66                     | 0.44              |
| 1:XA:1157:A:N3    | 1:XA:1157:A:H2'   | 2.31                     | 0.44              |
| 29:YF:18:ARG:HG2  | 29:YF:19:GLU:H    | 1.82                     | 0.44              |
| 1:QA:329:A:N6     | 1:QA:332:G:C2     | 2.85                     | 0.44              |
| 50:Y4:55:ARG:HE   | 50:Y4:56:VAL:N    | 2.16                     | 0.44              |
| 2:XB:178:ARG:NH2  | 8:XH:74:PRO:HB3   | 2.32                     | 0.44              |
| 36:YQ:55:VAL:HG23 | 36:YQ:64:ILE:HD11 | 1.98                     | 0.44              |
| 1:XA:316:G:OP2    | 1:XA:351:G:O2'    | 2.28                     | 0.44              |
| 27:RD:97:TYR:HE1  | 27:RD:103:ARG:HG3 | 1.83                     | 0.44              |
| 25:RA:2561:A:H2'  | 25:RA:2562:U:O4'  | 2.17                     | 0.44              |
| 30:RG:86:MET:HA   | 30:RG:87:PRO:HD2  | 1.74                     | 0.44              |
| 25:YA:1273:U:H5'  | 25:YA:1274:A:OP1  | 2.18                     | 0.44              |
| 25:RA:1766:U:H2'  | 25:RA:1767:C:C6   | 2.51                     | 0.44              |
| 26:YB:116:G:H5''  | 38:YS:55:ALA:HA   | 2.00                     | 0.44              |
| 12:XL:45:PRO:HG2  | 12:XL:49:ASN:O    | 2.17                     | 0.44              |
| 1:QA:406:G:H2'    | 1:QA:407:G:H8     | 1.82                     | 0.44              |
| 26:YB:42:C:O2     | 30:YG:93:THR:N    | 2.49                     | 0.44              |
| 2:QB:189:ASP:O    | 2:QB:191:ASP:N    | 2.50                     | 0.44              |
| 25:YA:1573:G:H2'  | 25:YA:1574:C:H5'  | 1.98                     | 0.44              |
| 25:YA:2512:C:H2'  | 25:YA:2513:G:O4'  | 2.17                     | 0.44              |
| 3:XC:179:ARG:NH1  | 3:XC:207:VAL:HG22 | 2.33                     | 0.44              |
| 25:YA:2252:G:C6   | 25:YA:2253:G:C5   | 3.05                     | 0.44              |
| 8:XH:21:LYS:O     | 8:XH:65:TYR:OH    | 2.20                     | 0.44              |
| 25:RA:512:G:OP1   | 25:RA:1234:U:O2'  | 2.28                     | 0.44              |
| 44:RY:7:VAL:HG21  | 44:RY:37:VAL:HG11 | 1.99                     | 0.44              |
| 25:RA:1246:A:H4'  | 29:RF:45:ARG:HH12 | 1.83                     | 0.44              |
| 25:YA:2689:U:P    | 25:YA:2719:G:H22  | 2.40                     | 0.44              |
| 24:QY:50:ILE:HG13 | 24:QY:51:TYR:CD1  | 2.53                     | 0.44              |
| 15:QO:26:GLU:OE2  | 15:QO:77:ARG:HD2  | 2.18                     | 0.44              |
| 40:RU:99:ALA:HB2  | 40:RU:106:PHE:CD1 | 2.52                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:YD:69:ARG:NH1   | 27:YD:128:GLY:O    | 2.46                     | 0.44              |
| 25:YA:27:G:N2      | 25:YA:512:G:H1'    | 2.33                     | 0.44              |
| 26:RB:11:C:OP2     | 46:R0:72:ARG:NH1   | 2.50                     | 0.44              |
| 27:RD:4:LYS:NZ     | 27:RD:20:ASP:HA    | 2.32                     | 0.44              |
| 25:RA:484:C:H2'    | 25:RA:485:C:H6     | 1.82                     | 0.44              |
| 50:Y4:5:ILE:HA     | 50:Y4:5:ILE:HD12   | 1.88                     | 0.44              |
| 25:RA:2394:C:OP1   | 35:RP:63:PRO:HD2   | 2.17                     | 0.44              |
| 1:XA:1498:U:H1'    | 1:XA:1499:A:OP2    | 2.17                     | 0.44              |
| 27:YD:206:LEU:HA   | 27:YD:206:LEU:HD23 | 1.82                     | 0.44              |
| 2:QB:163:PHE:HA    | 2:QB:185:ILE:HG13  | 1.98                     | 0.44              |
| 25:YA:1731:G:N1    | 25:YA:1732:A:N7    | 2.65                     | 0.44              |
| 12:QL:53:ARG:NH1   | 12:QL:92:ASP:OD2   | 2.40                     | 0.44              |
| 25:YA:1112:G:H2'   | 25:YA:1113:U:C6    | 2.52                     | 0.44              |
| 25:YA:1931:U:H2'   | 25:YA:1932:A:C8    | 2.53                     | 0.44              |
| 25:RA:2528:U:OP1   | 55:R9:30:PRO:HG2   | 2.17                     | 0.44              |
| 10:QJ:99:LYS:HD3   | 10:QJ:100:THR:H    | 1.83                     | 0.44              |
| 25:RA:139:G:H2'    | 25:RA:140:G:N7     | 2.33                     | 0.44              |
| 25:RA:218:A:H2     | 25:RA:235:U:H4'    | 1.82                     | 0.44              |
| 25:RA:2275:C:O2    | 36:RQ:83:MET:HG3   | 2.18                     | 0.44              |
| 1:XA:556:C:OP2     | 12:XL:20:LYS:NZ    | 2.43                     | 0.44              |
| 5:QE:92:LYS:HA     | 5:QE:93:PRO:HD2    | 1.89                     | 0.44              |
| 25:YA:270(N):G:O2' | 25:YA:270(O):U:H5' | 2.18                     | 0.44              |
| 3:QC:71:ALA:HB2    | 3:QC:115:LEU:HD13  | 1.99                     | 0.44              |
| 42:RW:29:LEU:HD21  | 42:RW:33:ARG:NH2   | 2.32                     | 0.44              |
| 25:RA:1129:A:HO2'  | 25:RA:2515:C:HO2'  | 1.66                     | 0.44              |
| 25:YA:2679:A:H4'   | 28:YE:165:VAL:HG11 | 1.98                     | 0.44              |
| 1:XA:135:C:N3      | 16:XP:1:MET:N      | 2.64                     | 0.44              |
| 8:QH:29:SER:HB3    | 8:QH:32:LYS:HG3    | 1.99                     | 0.44              |
| 50:Y4:13:ARG:N     | 50:Y4:24:THR:OG1   | 2.51                     | 0.44              |
| 25:RA:796:C:H2'    | 25:RA:797:C:C6     | 2.52                     | 0.44              |
| 25:RA:2543:G:H2'   | 25:RA:2544:G:C8    | 2.52                     | 0.44              |
| 25:RA:2280:G:C2    | 25:RA:2281:C:C6    | 3.04                     | 0.44              |
| 2:QB:21:ARG:NH2    | 2:QB:38:GLY:HA3    | 2.32                     | 0.44              |
| 20:XT:10:LEU:HD22  | 20:XT:11:SER:N     | 2.32                     | 0.44              |
| 1:QA:1473:A:H2'    | 1:QA:1474:G:C8     | 2.51                     | 0.44              |
| 45:YZ:135:GLU:H    | 45:YZ:135:GLU:HG2  | 1.60                     | 0.44              |
| 13:XM:93:ARG:HD3   | 13:XM:93:ARG:HA    | 1.64                     | 0.44              |
| 25:YA:1534:G:N2    | 25:YA:1537:C:N3    | 2.66                     | 0.44              |
| 45:YZ:40:ASP:HB3   | 45:YZ:43:GLU:HG3   | 2.00                     | 0.44              |
| 27:YD:144:ALA:HB3  | 27:YD:192:THR:HG23 | 2.00                     | 0.44              |
| 25:YA:523:C:H4'    | 25:YA:541:C:O2     | 2.16                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RA:1798:U:H5'  | 27:RD:259:THR:OG1 | 2.17                     | 0.44              |
| 34:YO:104:ARG:NE  | 39:YT:34:VAL:HG11 | 2.32                     | 0.44              |
| 13:XM:9:ILE:CG1   | 13:XM:10:PRO:N    | 2.81                     | 0.44              |
| 28:RE:63:LEU:HD12 | 28:RE:65:GLY:H    | 1.82                     | 0.44              |
| 40:RU:100:VAL:O   | 40:RU:101:ARG:HG2 | 2.17                     | 0.44              |
| 25:RA:2015:A:H5'  | 42:RW:92:ARG:HH21 | 1.83                     | 0.44              |
| 1:QA:1004:A:HO2'  | 1:QA:1005:A:P     | 2.40                     | 0.44              |
| 1:QA:354:G:C2     | 1:QA:355:C:C5     | 3.06                     | 0.44              |
| 27:RD:108:PRO:HA  | 27:RD:196:VAL:HA  | 1.99                     | 0.44              |
| 1:QA:1226:C:N4    | 13:QM:104:ARG:HD2 | 2.32                     | 0.44              |
| 2:QB:87:ARG:NH2   | 2:QB:233:SER:HB2  | 2.33                     | 0.44              |
| 1:QA:452:A:O2'    | 1:QA:453:A:O4'    | 2.33                     | 0.44              |
| 1:QA:1499:A:H1'   | 1:QA:1520:G:H5'   | 2.00                     | 0.44              |
| 22:QW:15:G:H2'    | 22:QW:59:A:H2     | 1.80                     | 0.44              |
| 1:QA:411:A:N9     | 1:QA:413:G:H1'    | 2.33                     | 0.44              |
| 1:XA:1008:C:H4'   | 1:XA:1008:C:OP1   | 2.18                     | 0.44              |
| 28:YE:11:MET:SD   | 28:YE:24:THR:HG22 | 2.58                     | 0.44              |
| 25:RA:1557:C:H5'' | 25:RA:1558:A:OP2  | 2.18                     | 0.44              |
| 1:XA:1376:U:H2'   | 1:XA:1377:A:C8    | 2.53                     | 0.44              |
| 25:YA:185:U:H2'   | 25:YA:186:G:H8    | 1.83                     | 0.44              |
| 25:RA:1999:C:H5'' | 25:RA:2723:C:O2'  | 2.17                     | 0.44              |
| 1:QA:1358:U:OP1   | 14:QN:35:ARG:HG2  | 2.17                     | 0.44              |
| 22:XV:33:U:N3     | 22:XV:36:U:OP2    | 2.42                     | 0.44              |
| 20:QT:32:ALA:O    | 20:QT:36:LEU:HB2  | 2.18                     | 0.44              |
| 25:YA:1800:C:OP2  | 27:YD:266:SER:OG  | 2.33                     | 0.44              |
| 34:YO:47:ILE:HG13 | 34:YO:48:PRO:HD2  | 1.98                     | 0.44              |
| 1:QA:719:C:O2'    | 18:QR:49:LYS:HB3  | 2.18                     | 0.44              |
| 16:XP:34:GLU:OE2  | 16:XP:55:ARG:HD3  | 2.17                     | 0.44              |
| 8:XH:42:GLU:HG3   | 8:XH:109:ILE:HD12 | 2.00                     | 0.44              |
| 6:QF:82:ARG:HB2   | 6:QF:85:VAL:HG22  | 2.00                     | 0.44              |
| 7:XG:97:GLN:HE21  | 7:XG:97:GLN:HB2   | 1.60                     | 0.44              |
| 3:XC:52:LEU:H     | 3:XC:52:LEU:HD23  | 1.82                     | 0.44              |
| 47:Y1:93:GLU:HG2  | 47:Y1:98:LEU:HD11 | 1.99                     | 0.44              |
| 25:RA:460:A:H2'   | 25:RA:461:C:O4'   | 2.16                     | 0.44              |
| 53:Y7:9:ARG:HH12  | 53:Y7:47:ARG:HH12 | 1.65                     | 0.44              |
| 25:RA:2748:A:O2'  | 31:RH:66:GLY:HA3  | 2.18                     | 0.44              |
| 50:Y4:5:ILE:HG13  | 50:Y4:6:HIS:HA    | 2.00                     | 0.44              |
| 13:XM:3:ARG:HA    | 13:XM:8:GLU:HA    | 1.99                     | 0.44              |
| 41:RV:40:LEU:HA   | 41:RV:40:LEU:HD23 | 1.86                     | 0.44              |
| 25:YA:828:U:H4'   | 25:YA:831:G:N1    | 2.32                     | 0.44              |
| 25:YA:2287:A:O2'  | 25:YA:2288:A:H5'' | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:YH:52:VAL:O     | 31:YH:65:HIS:NE2   | 2.42                     | 0.44              |
| 41:YV:71:LEU:H     | 41:YV:86:GLY:CA    | 2.30                     | 0.44              |
| 4:QD:9:CYS:SG      | 4:QD:32:ALA:HB2    | 2.58                     | 0.44              |
| 1:QA:316:G:C2      | 1:QA:338:A:C2      | 3.06                     | 0.44              |
| 4:XD:3:ARG:NE      | 4:XD:118:ARG:CD    | 2.79                     | 0.44              |
| 25:RA:907:U:O2'    | 36:RQ:101:ARG:NH2  | 2.33                     | 0.44              |
| 34:RO:68:GLU:HB3   | 34:RO:78:ARG:HB2   | 1.98                     | 0.44              |
| 25:RA:1911:U:H2'   | 25:RA:1918:A:N1    | 2.33                     | 0.44              |
| 2:QB:184:VAL:HG12  | 2:QB:197:VAL:HG13  | 2.00                     | 0.44              |
| 26:YB:81:G:C6      | 26:YB:82:G:C5      | 3.05                     | 0.44              |
| 25:RA:614(A):U:H6  | 25:RA:614(A):U:H3' | 1.83                     | 0.44              |
| 1:QA:1326:C:OP2    | 21:QU:6:ARG:HD3    | 2.18                     | 0.44              |
| 1:XA:1300:G:O2'    | 1:XA:1301:U:P      | 2.76                     | 0.44              |
| 1:XA:832:C:H2'     | 1:XA:833:U:O4'     | 2.18                     | 0.44              |
| 25:RA:2313:C:H2'   | 25:RA:2314:C:H6    | 1.82                     | 0.44              |
| 25:RA:2696:U:H2'   | 25:RA:2697:G:H8    | 1.83                     | 0.44              |
| 44:YY:56:PRO:O     | 44:YY:57:GLN:HB2   | 2.17                     | 0.44              |
| 1:QA:1117:G:H4'    | 9:QI:104:ARG:HD2   | 1.98                     | 0.44              |
| 25:YA:746:A:C6     | 25:YA:2611:U:H5''  | 2.53                     | 0.44              |
| 20:QT:25:ARG:HG2   | 20:QT:29:LYS:NZ    | 2.33                     | 0.44              |
| 25:RA:1476:C:H2'   | 25:RA:1477:A:H8    | 1.82                     | 0.44              |
| 26:RB:44:G:H5''    | 26:RB:45:A:OP1     | 2.18                     | 0.44              |
| 25:YA:2698:U:H2'   | 25:YA:2699:C:C6    | 2.53                     | 0.44              |
| 22:QW:41:C:H2'     | 22:QW:42:G:C8      | 2.52                     | 0.44              |
| 12:QL:110:VAL:HG23 | 12:QL:120:TYR:HB3  | 2.00                     | 0.44              |
| 1:QA:1244:C:H2'    | 1:QA:1245:A:C8     | 2.53                     | 0.44              |
| 25:YA:184:C:O2'    | 25:YA:217:G:N3     | 2.50                     | 0.44              |
| 32:RI:12:LEU:HG    | 32:RI:19:VAL:HG11  | 2.00                     | 0.44              |
| 2:QB:178:ARG:HH22  | 8:QH:74:PRO:HB3    | 1.83                     | 0.44              |
| 1:XA:262:A:C6      | 1:XA:263:A:C6      | 3.04                     | 0.44              |
| 34:YO:8:LEU:HB2    | 34:YO:19:ILE:HG13  | 2.00                     | 0.44              |
| 25:RA:1639:U:H4'   | 25:RA:2699:C:H4'   | 2.00                     | 0.44              |
| 50:Y4:5:ILE:HA     | 50:Y4:6:HIS:HA     | 1.78                     | 0.44              |
| 28:RE:47:VAL:O     | 28:RE:48:GLN:C     | 2.56                     | 0.44              |
| 1:QA:1347:G:C1'    | 1:QA:1348:U:OP2    | 2.65                     | 0.44              |
| 1:XA:1223:C:H5''   | 1:XA:1224:G:H5''   | 1.99                     | 0.44              |
| 27:YD:35:LYS:HZ1   | 27:YD:104:TYR:HB2  | 1.83                     | 0.44              |
| 38:YS:62:LYS:HD3   | 38:YS:97:ARG:NH1   | 2.33                     | 0.44              |
| 25:YA:483:A:H4'    | 44:YY:49:VAL:O     | 2.18                     | 0.44              |
| 25:RA:583:G:H5''   | 40:RU:10:ARG:HH12  | 1.83                     | 0.44              |
| 2:XB:15:VAL:HG21   | 2:XB:209:ARG:HB3   | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2287:A:H62   | 25:RA:2344:U:H3    | 1.63                     | 0.44              |
| 25:RA:1096:A:C5    | 25:RA:1097:U:H1'   | 2.53                     | 0.44              |
| 6:XF:86:ARG:O      | 6:XF:87:ARG:HG2    | 2.18                     | 0.44              |
| 6:XF:97:PHE:HD2    | 18:XR:31:LEU:HD11  | 1.83                     | 0.44              |
| 15:XO:70:LEU:HD11  | 15:XO:77:ARG:HG3   | 1.98                     | 0.44              |
| 25:RA:878:A:H3'    | 25:RA:879:G:C8     | 2.52                     | 0.44              |
| 1:XA:46:G:O2'      | 1:XA:365:U:H1'     | 2.18                     | 0.44              |
| 27:YD:260:ARG:NH1  | 27:YD:267:SER:OG   | 2.51                     | 0.44              |
| 1:XA:1252:A:H61    | 1:XA:1285:A:H61    | 1.65                     | 0.44              |
| 25:RA:1810:A:H2'   | 25:RA:1811:G:O4'   | 2.18                     | 0.44              |
| 29:RF:34:TRP:HB2   | 35:RP:6:LEU:HD12   | 1.99                     | 0.44              |
| 29:RF:140:LEU:HD13 | 29:RF:170:LEU:HD21 | 1.98                     | 0.44              |
| 25:RA:2294:C:P     | 38:RS:89:ARG:HH22  | 2.41                     | 0.44              |
| 1:XA:1278:U:H5'    | 1:XA:1279:A:O4'    | 2.18                     | 0.44              |
| 25:YA:55:G:O2'     | 25:YA:127:A:N1     | 2.37                     | 0.44              |
| 1:QA:524:G:H2'     | 1:QA:525:C:C6      | 2.53                     | 0.44              |
| 25:YA:705:A:O3'    | 27:YD:7:LYS:HD2    | 2.17                     | 0.44              |
| 6:QF:76:ALA:O      | 6:QF:80:ARG:HG3    | 2.17                     | 0.44              |
| 46:R0:11:ARG:O     | 46:R0:14:ARG:NH1   | 2.37                     | 0.44              |
| 3:XC:164:ARG:HG2   | 3:XC:165:THR:H     | 1.83                     | 0.44              |
| 12:QL:85:ILE:HA    | 12:QL:85:ILE:HD12  | 1.85                     | 0.44              |
| 32:YI:95:LYS:HE2   | 32:YI:95:LYS:HB3   | 1.86                     | 0.44              |
| 6:XF:69:GLU:CD     | 6:XF:69:GLU:H      | 2.21                     | 0.44              |
| 30:YG:55:LYS:O     | 30:YG:59:GLU:HB2   | 2.17                     | 0.44              |
| 25:YA:1802:A:N1    | 25:YA:1822:G:H1'   | 2.32                     | 0.44              |
| 25:RA:2109:U:H2'   | 25:RA:2110:G:C8    | 2.53                     | 0.44              |
| 1:QA:778:G:H2'     | 1:QA:779:C:O4'     | 2.18                     | 0.44              |
| 44:YY:97:ARG:NH2   | 44:YY:98:VAL:HB    | 2.24                     | 0.44              |
| 35:RP:62:LEU:HD21  | 54:R8:30:ARG:HD2   | 1.99                     | 0.44              |
| 21:XU:2:GLY:O      | 21:XU:4:GLY:N      | 2.51                     | 0.44              |
| 9:XI:29:ASN:HB3    | 9:XI:30:GLY:H      | 1.65                     | 0.44              |
| 32:RI:92:VAL:HB    | 32:RI:120:ILE:HB   | 1.99                     | 0.44              |
| 25:YA:2414:G:H21   | 35:YP:67:MET:HE1   | 1.83                     | 0.44              |
| 35:RP:97:PRO:HD3   | 35:RP:126:VAL:O    | 2.18                     | 0.44              |
| 4:XD:111:ALA:HB1   | 4:XD:116:GLN:HG2   | 2.00                     | 0.44              |
| 25:YA:1085:A:O2'   | 25:YA:1086:A:OP1   | 2.32                     | 0.44              |
| 1:QA:452:A:O2'     | 1:QA:453:A:O5'     | 2.36                     | 0.44              |
| 25:YA:46:C:H2'     | 25:YA:47:C:C6      | 2.53                     | 0.44              |
| 25:RA:2746:U:H4'   | 31:RH:138:LYS:HG3  | 1.99                     | 0.44              |
| 1:QA:749:C:H2'     | 1:QA:750:G:H8      | 1.83                     | 0.44              |
| 1:QA:1007:C:H3'    | 1:QA:1008:C:H5''   | 1.98                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:RH:86:GLU:N     | 31:RH:86:GLU:OE1   | 2.51                     | 0.44              |
| 48:Y2:47:ASN:HB2   | 48:Y2:48:HIS:H     | 1.55                     | 0.44              |
| 1:QA:1343:G:H2'    | 1:QA:1344:C:C6     | 2.53                     | 0.44              |
| 25:YA:815:C:H2'    | 25:YA:816:C:H6     | 1.82                     | 0.44              |
| 25:RA:654(A):G:C6  | 25:RA:654(U):A:C2  | 3.06                     | 0.44              |
| 29:YF:140:LEU:HD13 | 29:YF:170:LEU:HD21 | 1.99                     | 0.44              |
| 1:QA:503:C:OP2     | 12:QL:116:SER:HB3  | 2.18                     | 0.44              |
| 4:QD:102:ASP:OD2   | 4:QD:103:ASN:N     | 2.51                     | 0.44              |
| 27:RD:142:VAL:HG23 | 27:RD:193:VAL:HA   | 1.99                     | 0.44              |
| 26:RB:113:C:H4'    | 38:RS:46:VAL:HG22  | 2.00                     | 0.44              |
| 25:YA:499:U:H2'    | 25:YA:500:G:C8     | 2.53                     | 0.44              |
| 1:QA:1239:A:H4'    | 1:QA:1240:U:H5''   | 2.00                     | 0.44              |
| 2:XB:135:GLN:HG3   | 2:XB:136:VAL:HG23  | 1.98                     | 0.44              |
| 24:XY:41:THR:O     | 24:XY:81:GLY:HA2   | 2.18                     | 0.44              |
| 1:XA:1347:G:C8     | 9:XI:107:ARG:HB3   | 2.53                     | 0.44              |
| 17:XQ:45:HIS:HB2   | 17:XQ:65:ILE:HD12  | 1.98                     | 0.44              |
| 1:XA:147:G:H1      | 1:XA:175:C:H42     | 1.65                     | 0.44              |
| 1:XA:175:C:H4'     | 20:XT:25:ARG:NH1   | 2.33                     | 0.44              |
| 25:RA:105:C:O2'    | 44:RY:2:ARG:NE     | 2.51                     | 0.44              |
| 1:XA:1225:A:H2'    | 1:XA:1225:A:N3     | 2.32                     | 0.44              |
| 17:QQ:57:VAL:HG12  | 17:QQ:76:LEU:HA    | 2.00                     | 0.44              |
| 1:XA:920:U:H2'     | 1:XA:921:U:C6      | 2.52                     | 0.44              |
| 32:YI:77:LEU:HB2   | 32:YI:142:VAL:HG21 | 1.79                     | 0.43              |
| 54:Y8:25:MET:SD    | 54:Y8:47:LYS:HG2   | 2.58                     | 0.43              |
| 28:RE:61:ARG:N     | 28:RE:62:PRO:CD    | 2.81                     | 0.43              |
| 25:RA:2580:U:H4'   | 28:RE:130:GLY:CA   | 2.41                     | 0.43              |
| 25:RA:659:C:H2'    | 25:RA:660:G:C8     | 2.51                     | 0.43              |
| 1:XA:1363:C:H5'    | 1:XA:1363(A):A:OP1 | 2.18                     | 0.43              |
| 45:RZ:171:ILE:HD13 | 45:RZ:172:ALA:N    | 2.33                     | 0.43              |
| 35:RP:52:GLU:OE1   | 35:RP:53:GLY:N     | 2.51                     | 0.43              |
| 29:YF:28:ILE:O     | 29:YF:30:PRO:HD3   | 2.17                     | 0.43              |
| 54:R8:54:GLU:OE2   | 54:R8:55:ALA:N     | 2.50                     | 0.43              |
| 52:Y6:12:GLU:HA    | 52:Y6:24:GLU:HG2   | 2.00                     | 0.43              |
| 35:RP:126:VAL:HG22 | 35:RP:145:PRO:HG2  | 2.00                     | 0.43              |
| 28:RE:8:LYS:O      | 28:RE:10:GLY:N     | 2.50                     | 0.43              |
| 1:XA:827:U:H3      | 1:XA:872:A:H62     | 1.66                     | 0.43              |
| 25:YA:590:A:H2'    | 25:YA:591:C:C6     | 2.53                     | 0.43              |
| 25:YA:1931:U:H2'   | 25:YA:1932:A:H8    | 1.82                     | 0.43              |
| 1:QA:1289:A:H2'    | 1:QA:1290:G:H5'    | 2.00                     | 0.43              |
| 25:RA:1675:C:H2'   | 25:RA:1676:A:O4'   | 2.17                     | 0.43              |
| 35:YP:101:VAL:HG21 | 35:YP:108:LYS:HG2  | 1.99                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:XJ:57:LYS:HA    | 10:XJ:57:LYS:HD3  | 1.81                     | 0.43              |
| 25:RA:1988:C:H2'   | 25:RA:1989:G:C8   | 2.52                     | 0.43              |
| 28:YE:23:VAL:O     | 28:YE:24:THR:OG1  | 2.34                     | 0.43              |
| 25:RA:388:G:H4'    | 47:R1:25:LYS:HE2  | 2.00                     | 0.43              |
| 54:R8:34:TRP:CG    | 54:R8:35:GLN:N    | 2.83                     | 0.43              |
| 25:RA:389:G:N1     | 35:RP:71:VAL:HG12 | 2.33                     | 0.43              |
| 38:RS:110:LEU:HB3  | 38:RS:111:GLU:H   | 1.51                     | 0.43              |
| 25:YA:92:G:H2'     | 25:YA:93:C:C6     | 2.53                     | 0.43              |
| 25:RA:606:U:H4'    | 25:RA:658:C:H4'   | 2.00                     | 0.43              |
| 2:XB:93:VAL:HG11   | 2:XB:97:TRP:CD1   | 2.53                     | 0.43              |
| 25:YA:39:C:O2      | 29:YF:46:ARG:NH2  | 2.50                     | 0.43              |
| 1:XA:262:A:H2'     | 1:XA:263:A:C8     | 2.53                     | 0.43              |
| 12:XL:47:LYS:HB3   | 12:XL:48:PRO:HD3  | 2.00                     | 0.43              |
| 30:YG:53:LEU:HG    | 30:YG:90:LEU:HD21 | 2.00                     | 0.43              |
| 1:QA:1412:C:H2'    | 1:QA:1413:A:C8    | 2.53                     | 0.43              |
| 47:R1:62:VAL:HG23  | 47:R1:63:ALA:O    | 2.18                     | 0.43              |
| 42:YW:20:VAL:HG22  | 42:YW:47:VAL:HG21 | 2.00                     | 0.43              |
| 25:RA:2537:U:H2'   | 25:RA:2538:C:C6   | 2.53                     | 0.43              |
| 51:Y5:16:ARG:NH1   | 51:Y5:17:ASP:OD1  | 2.51                     | 0.43              |
| 14:YN:3:ARG:O      | 14:YN:7:ILE:HG23  | 2.18                     | 0.43              |
| 25:RA:706:A:H2'    | 25:RA:707:G:O4'   | 2.18                     | 0.43              |
| 18:XR:41:LYS:HB3   | 18:XR:41:LYS:HE3  | 1.84                     | 0.43              |
| 25:YA:774:A:H2'    | 25:YA:774:A:N3    | 2.33                     | 0.43              |
| 1:QA:1388:C:H2'    | 1:QA:1389:C:C6    | 2.53                     | 0.43              |
| 25:RA:2116:G:N2    | 25:RA:2165:G:O6   | 2.51                     | 0.43              |
| 25:YA:30:G:H2'     | 25:YA:31:C:C6     | 2.53                     | 0.43              |
| 32:YI:56:LYS:HA    | 32:YI:59:ALA:HB3  | 1.99                     | 0.43              |
| 28:RE:79:ARG:O     | 28:RE:80:GLU:HG3  | 2.18                     | 0.43              |
| 1:QA:1502:A:H2     | 1:QA:1505:G:N1    | 2.03                     | 0.43              |
| 22:QV:2:G:C2'      | 22:QV:3:C:O5'     | 2.66                     | 0.43              |
| 52:R6:14:THR:HG1   | 52:R6:15:GLU:H    | 1.61                     | 0.43              |
| 39:RT:125:ARG:HA   | 39:RT:125:ARG:HD3 | 1.78                     | 0.43              |
| 35:RP:39:LYS:HG3   | 35:RP:45:LEU:HD22 | 1.99                     | 0.43              |
| 15:QO:23:GLY:O     | 15:QO:27:VAL:HB   | 2.18                     | 0.43              |
| 3:QC:7:PRO:O       | 3:QC:11:ARG:HG2   | 2.18                     | 0.43              |
| 25:YA:768:G:O2'    | 25:YA:1379:A:N6   | 2.50                     | 0.43              |
| 25:YA:1047:G:H2'   | 25:YA:1110:G:N1   | 2.33                     | 0.43              |
| 35:YP:21:ARG:HB3   | 35:YP:22:GLY:H    | 1.66                     | 0.43              |
| 25:YA:270(G):C:H2' | 25:YA:270(H):C:C6 | 2.53                     | 0.43              |
| 1:QA:110:C:O2'     | 16:QP:25:ARG:O    | 2.33                     | 0.43              |
| 25:YA:2684:U:OP1   | 39:YT:53:ARG:HD3  | 2.18                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:RA:1667:G:O2'   | 25:RA:1991:U:O4   | 2.24                     | 0.43              |
| 34:RO:10:VAL:HG22  | 34:RO:17:ARG:O    | 2.19                     | 0.43              |
| 25:RA:2330:G:H2'   | 25:RA:2331:G:O4'  | 2.18                     | 0.43              |
| 1:XA:892:A:O2'     | 1:XA:1415:G:H4'   | 2.19                     | 0.43              |
| 25:YA:2345:G:N3    | 25:YA:2381:C:H2'  | 2.33                     | 0.43              |
| 33:YN:46:VAL:HG13  | 33:YN:48:MET:HG3  | 2.00                     | 0.43              |
| 25:YA:919:G:N2     | 25:YA:2269:A:OP2  | 2.49                     | 0.43              |
| 25:YA:1149:G:H2'   | 25:YA:1150:C:C6   | 2.53                     | 0.43              |
| 25:YA:1895:C:H2'   | 25:YA:1896:G:O4'  | 2.18                     | 0.43              |
| 1:XA:939:G:H5''    | 7:XG:102:ARG:NH2  | 2.32                     | 0.43              |
| 40:YU:52:ARG:HB3   | 40:YU:52:ARG:NH1  | 2.33                     | 0.43              |
| 32:RI:48:GLU:HA    | 32:RI:51:ILE:HB   | 2.00                     | 0.43              |
| 1:QA:392:G:H2'     | 1:QA:393:A:H8     | 1.83                     | 0.43              |
| 25:YA:273(F):C:H3' | 25:YA:274:G:H5''  | 1.99                     | 0.43              |
| 1:XA:540:G:C6      | 1:XA:541:G:C5     | 3.07                     | 0.43              |
| 25:YA:1009:A:N3    | 25:YA:1153:C:O2'  | 2.44                     | 0.43              |
| 25:YA:987:G:C2'    | 25:YA:988:A:C5'   | 2.86                     | 0.43              |
| 44:RY:17:SER:CB    | 44:RY:71:LYS:HB3  | 2.48                     | 0.43              |
| 1:QA:664:G:N2      | 1:QA:741:G:H1     | 2.02                     | 0.43              |
| 19:QS:71:LEU:O     | 19:QS:73:GLU:N    | 2.51                     | 0.43              |
| 25:YA:6:A:O5'      | 25:YA:6:A:H8      | 2.01                     | 0.43              |
| 44:YY:19:LYS:HE3   | 44:YY:71:LYS:NZ   | 2.28                     | 0.43              |
| 25:YA:1566:A:OP1   | 27:YD:211:ARG:NH1 | 2.50                     | 0.43              |
| 35:RP:52:GLU:HB2   | 35:RP:53:GLY:H    | 1.49                     | 0.43              |
| 1:QA:349:A:C5'     | 1:QA:350:G:OP2    | 2.66                     | 0.43              |
| 25:YA:2406:U:C4    | 35:YP:72:PRO:HD2  | 2.53                     | 0.43              |
| 25:YA:2414:G:H21   | 35:YP:67:MET:CE   | 2.31                     | 0.43              |
| 25:RA:2199:A:C8    | 25:RA:2225:A:N6   | 2.86                     | 0.43              |
| 1:QA:1064:G:H1'    | 1:QA:1066:C:C6    | 2.54                     | 0.43              |
| 25:RA:2231:C:H2'   | 25:RA:2232:U:O4'  | 2.18                     | 0.43              |
| 7:XG:113:GLU:H     | 7:XG:113:GLU:HG2  | 1.57                     | 0.43              |
| 1:XA:1327:C:OP2    | 21:XU:12:LYS:NZ   | 2.51                     | 0.43              |
| 9:XI:20:ARG:HB2    | 9:XI:60:ASP:HB2   | 1.99                     | 0.43              |
| 29:YF:117:ARG:HD3  | 29:YF:117:ARG:HA  | 1.71                     | 0.43              |
| 25:RA:1906:G:O2'   | 25:RA:1907:G:H5'  | 2.18                     | 0.43              |
| 29:RF:46:ARG:HH11  | 29:RF:46:ARG:HG2  | 1.83                     | 0.43              |
| 19:QS:16:LEU:HA    | 19:QS:19:VAL:HG12 | 1.98                     | 0.43              |
| 25:RA:1484:G:H2'   | 25:RA:1485:G:H5'' | 2.00                     | 0.43              |
| 25:YA:528:A:N3     | 25:YA:528:A:H2'   | 2.33                     | 0.43              |
| 28:RE:117:MET:HG2  | 28:RE:117:MET:O   | 2.19                     | 0.43              |
| 1:XA:1324:A:C4'    | 1:XA:1362:C:H4'   | 2.49                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:RA:2769:C:H2'   | 25:RA:2770:G:H8    | 1.83                     | 0.43              |
| 1:QA:697:U:H3'     | 1:QA:698:G:H8      | 1.84                     | 0.43              |
| 12:QL:71:PRO:HD2   | 12:QL:102:ARG:HD2  | 2.00                     | 0.43              |
| 25:RA:2390:U:O2'   | 25:RA:2391:G:H5'   | 2.19                     | 0.43              |
| 6:QF:35:ALA:HA     | 6:QF:67:MET:HB3    | 2.00                     | 0.43              |
| 25:YA:2815:C:H5'   | 51:Y5:29:THR:HG21  | 1.99                     | 0.43              |
| 1:XA:667:G:H4'     | 15:XO:51:HIS:ND1   | 2.32                     | 0.43              |
| 25:RA:2747:G:O6    | 25:RA:2755:C:H5'   | 2.18                     | 0.43              |
| 8:XH:99:GLU:OE1    | 8:XH:99:GLU:N      | 2.51                     | 0.43              |
| 54:R8:38:GLY:O     | 54:R8:41:ILE:HG22  | 2.18                     | 0.43              |
| 1:QA:860:A:H2'     | 1:QA:861:G:O4'     | 2.18                     | 0.43              |
| 32:YI:140:LEU:HA   | 32:YI:140:LEU:HD12 | 1.87                     | 0.43              |
| 25:RA:2635:C:OP1   | 28:RE:78:LEU:HD13  | 2.17                     | 0.43              |
| 45:YZ:150:LEU:HG   | 45:YZ:171:ILE:HG22 | 2.00                     | 0.43              |
| 32:YI:144:VAL:C    | 32:YI:145:VAL:CG1  | 2.83                     | 0.43              |
| 41:YV:71:LEU:H     | 41:YV:86:GLY:HA3   | 1.83                     | 0.43              |
| 25:RA:1688:U:H1'   | 25:RA:1701:A:C6    | 2.54                     | 0.43              |
| 24:XY:91:TYR:O     | 24:XY:91:TYR:CG    | 2.70                     | 0.43              |
| 20:XT:77:ALA:O     | 20:XT:81:LYS:HB2   | 2.18                     | 0.43              |
| 32:RI:145:VAL:HG12 | 32:RI:146:ALA:N    | 2.33                     | 0.43              |
| 25:RA:1721:G:H8    | 25:RA:1741:A:N6    | 2.16                     | 0.43              |
| 25:RA:2287:A:H2    | 25:RA:2346:A:H62   | 1.65                     | 0.43              |
| 25:RA:1085:A:O2'   | 25:RA:1086:A:OP1   | 2.35                     | 0.43              |
| 1:QA:1301:U:O4     | 1:QA:1303:C:N1     | 2.51                     | 0.43              |
| 2:XB:6:THR:HG23    | 2:XB:217:ARG:HB3   | 2.00                     | 0.43              |
| 32:RI:2:LYS:HA     | 32:RI:20:ASP:HA    | 1.99                     | 0.43              |
| 25:YA:635:C:H2'    | 25:YA:636:G:O4'    | 2.17                     | 0.43              |
| 25:RA:2140:C:H42   | 25:RA:2151:G:H1    | 1.66                     | 0.43              |
| 25:YA:754:C:H2'    | 25:YA:755:C:H6     | 1.84                     | 0.43              |
| 25:YA:1843:C:H2'   | 25:YA:1844:C:H6    | 1.84                     | 0.43              |
| 3:XC:153:VAL:HG22  | 3:XC:198:VAL:HG22  | 1.99                     | 0.43              |
| 22:XW:5:G:N2       | 22:XW:69:C:O2      | 2.51                     | 0.43              |
| 32:YI:4:ILE:HG12   | 32:YI:18:VAL:HG22  | 2.00                     | 0.43              |
| 25:YA:1328:G:H8    | 25:YA:1328:G:O5'   | 2.02                     | 0.43              |
| 25:YA:2755:C:O2'   | 25:YA:2756:U:H2'   | 2.19                     | 0.43              |
| 25:YA:1819:A:H4'   | 25:YA:1820:U:O5'   | 2.19                     | 0.43              |
| 25:YA:2247:A:H2'   | 25:YA:2248:C:C6    | 2.53                     | 0.43              |
| 1:QA:1280:A:H5'    | 1:QA:1281:U:OP2    | 2.18                     | 0.43              |
| 44:RY:95:LYS:O     | 44:RY:95:LYS:HD3   | 2.18                     | 0.43              |
| 31:RH:10:PRO:HB2   | 31:RH:11:VAL:H     | 1.61                     | 0.43              |
| 28:RE:48:GLN:O     | 28:RE:49:LEU:HD13  | 2.13                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:2633:G:H1'   | 28:YE:62:PRO:HG3   | 2.01                     | 0.43              |
| 28:YE:60:ASN:O     | 28:YE:62:PRO:HD3   | 2.18                     | 0.43              |
| 25:YA:833:U:H2'    | 25:YA:834:C:C6     | 2.54                     | 0.43              |
| 15:QO:36:ILE:HG23  | 15:QO:56:LEU:HD11  | 2.00                     | 0.43              |
| 1:QA:321:A:C8      | 1:QA:328:C:O2      | 2.71                     | 0.43              |
| 22:XW:16:C:H4'     | 22:XW:60:U:H4'     | 2.00                     | 0.43              |
| 9:XI:103:THR:HG22  | 9:XI:105:ASP:H     | 1.83                     | 0.43              |
| 25:RA:1020:A:N1    | 25:RA:1141:U:H2'   | 2.33                     | 0.43              |
| 7:QG:16:LEU:HD21   | 9:QI:42:ARG:HA     | 2.00                     | 0.43              |
| 30:YG:114:ILE:HG12 | 30:YG:140:ILE:HD13 | 2.00                     | 0.43              |
| 41:RV:5:VAL:HG23   | 41:RV:37:VAL:HG11  | 2.00                     | 0.43              |
| 25:RA:2208:A:N3    | 25:RA:2219:G:C2    | 2.87                     | 0.43              |
| 19:XS:5:LEU:HD12   | 19:XS:5:LEU:H      | 1.84                     | 0.43              |
| 1:XA:1326:C:H2'    | 1:XA:1327:C:C6     | 2.52                     | 0.43              |
| 1:XA:1300:G:HO2'   | 1:XA:1301:U:P      | 2.42                     | 0.43              |
| 30:RG:82:LEU:HA    | 30:RG:86:MET:SD    | 2.57                     | 0.43              |
| 1:XA:302:G:O2'     | 1:XA:556:C:H5''    | 2.18                     | 0.43              |
| 25:YA:270(F):U:H2' | 25:YA:270(G):C:H6  | 1.84                     | 0.43              |
| 1:XA:392:G:H2'     | 1:XA:393:A:H8      | 1.83                     | 0.43              |
| 1:QA:1175:G:H2'    | 1:QA:1176:A:C8     | 2.52                     | 0.43              |
| 25:RA:2183:C:H2'   | 25:RA:2184:G:C8    | 2.53                     | 0.43              |
| 1:XA:1423:G:OP1    | 34:YO:49:ARG:NH2   | 2.51                     | 0.43              |
| 7:XG:47:CYS:O      | 7:XG:50:ILE:HB     | 2.18                     | 0.43              |
| 1:XA:601:C:H42     | 1:XA:637:G:H1      | 1.67                     | 0.43              |
| 25:RA:28:A:H1'     | 25:RA:513:A:C2     | 2.53                     | 0.43              |
| 25:RA:943:U:C4     | 25:RA:944:G:N7     | 2.86                     | 0.43              |
| 48:R2:42:GLY:O     | 48:R2:44:LEU:N     | 2.40                     | 0.43              |
| 1:QA:142:G:H2'     | 1:QA:143:A:H8      | 1.83                     | 0.43              |
| 38:YS:110:LEU:HB3  | 38:YS:111:GLU:H    | 1.52                     | 0.43              |
| 13:XM:59:TYR:O     | 13:XM:63:THR:OG1   | 2.27                     | 0.43              |
| 1:XA:1067:A:O2'    | 1:XA:1094:G:H5'    | 2.17                     | 0.43              |
| 25:YA:1769:G:O2'   | 25:YA:1958:C:OP1   | 2.24                     | 0.43              |
| 1:QA:1429:C:H2'    | 1:QA:1430:C:H6     | 1.84                     | 0.43              |
| 16:QP:43:LYS:HG2   | 16:QP:48:TRP:CD2   | 2.53                     | 0.43              |
| 42:RW:5:ALA:HB3    | 42:RW:54:ALA:HB2   | 2.00                     | 0.43              |
| 1:XA:1065:U:O2'    | 1:XA:1066:C:OP2    | 2.32                     | 0.43              |
| 10:XJ:33:GLN:H     | 10:XJ:75:ILE:HD11  | 1.83                     | 0.43              |
| 1:XA:1250:A:H4'    | 9:XI:68:GLY:N      | 2.33                     | 0.43              |
| 25:YA:2839:G:H5'   | 37:YR:46:GLY:HA2   | 2.00                     | 0.43              |
| 25:YA:2745:C:C4    | 25:YA:2746:U:C4    | 3.07                     | 0.43              |
| 25:RA:271:A:OP1    | 47:R1:97:LEU:HD22  | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:RF:129:PHE:CG   | 29:RF:163:VAL:HG21 | 2.53                     | 0.43              |
| 1:XA:443:C:H2'     | 1:XA:444:C:H6      | 1.82                     | 0.43              |
| 25:RA:716:A:C2     | 25:RA:717:G:H1'    | 2.52                     | 0.43              |
| 37:YR:116:LEU:HA   | 37:YR:116:LEU:HD23 | 1.83                     | 0.43              |
| 2:QB:135:GLN:HB2   | 2:QB:135:GLN:HE21  | 1.70                     | 0.43              |
| 25:YA:2556:C:H2'   | 25:YA:2557:G:O4'   | 2.18                     | 0.43              |
| 1:XA:1190:G:OP1    | 3:XC:5:ILE:HG23    | 2.16                     | 0.43              |
| 22:QW:12:G:H2'     | 22:QW:13:C:C6      | 2.54                     | 0.43              |
| 25:YA:2109:U:H2'   | 25:YA:2110:G:H8    | 1.83                     | 0.43              |
| 27:YD:10:THR:OG1   | 27:YD:13:ARG:HB2   | 2.18                     | 0.43              |
| 25:YA:836:G:C5     | 25:YA:837:C:C4     | 3.07                     | 0.43              |
| 14:YN:41:ARG:HG3   | 14:YN:42:ILE:N     | 2.33                     | 0.43              |
| 44:YY:84:ARG:NH2   | 44:YY:97:ARG:HB2   | 2.33                     | 0.43              |
| 2:XB:163:PHE:HA    | 2:XB:185:ILE:HG13  | 2.01                     | 0.43              |
| 1:XA:954:G:H2'     | 1:XA:955:U:O4'     | 2.18                     | 0.43              |
| 29:YF:125:LEU:HD12 | 29:YF:196:LEU:HD23 | 2.00                     | 0.43              |
| 23:XX:21:A2M:HM'2  | 23:XX:21:A2M:H1'   | 1.82                     | 0.43              |
| 3:QC:40:ARG:NH2    | 3:QC:55:VAL:O      | 2.51                     | 0.43              |
| 31:RH:44:VAL:HG22  | 31:RH:51:ARG:NH1   | 2.33                     | 0.43              |
| 25:RA:48:G:N2      | 25:RA:49:A:N1      | 2.67                     | 0.43              |
| 25:RA:128:C:O2'    | 25:RA:129:C:OP1    | 2.30                     | 0.43              |
| 26:RB:30:C:H2'     | 26:RB:31:C:O4'     | 2.19                     | 0.43              |
| 46:Y0:3:HIS:O      | 46:Y0:4:LYS:HG3    | 2.19                     | 0.43              |
| 41:RV:2:PHE:HD2    | 41:RV:42:GLY:HA2   | 1.82                     | 0.43              |
| 28:RE:154:LYS:HE3  | 28:RE:154:LYS:HA   | 1.99                     | 0.43              |
| 1:QA:56:U:H2'      | 1:QA:57:G:C8       | 2.53                     | 0.43              |
| 11:QK:29:ILE:HB    | 11:QK:44:SER:HB3   | 1.99                     | 0.43              |
| 25:YA:593:G:H1'    | 54:Y8:4:MET:HE1    | 2.00                     | 0.43              |
| 35:RP:98:GLU:O     | 35:RP:101:VAL:HG12 | 2.18                     | 0.43              |
| 25:YA:829:A:N7     | 25:YA:2248:C:H5'   | 2.33                     | 0.43              |
| 35:YP:49:ARG:HD2   | 54:Y8:58:ILE:CG2   | 2.49                     | 0.43              |
| 11:QK:15:ALA:HB2   | 11:QK:76:GLY:O     | 2.19                     | 0.43              |
| 19:QS:48:THR:HG22  | 19:QS:61:TYR:HD1   | 1.82                     | 0.43              |
| 43:YX:8:ILE:O      | 48:Y2:36:ARG:NH2   | 2.52                     | 0.43              |
| 1:XA:1221:G:OP1    | 1:XA:1320:C:N4     | 2.49                     | 0.43              |
| 1:XA:966:G:O2'     | 9:XI:127:LYS:O     | 2.37                     | 0.43              |
| 25:RA:1813:G:H1'   | 27:RD:50:THR:OG1   | 2.19                     | 0.43              |
| 39:YT:65:LYS:HE3   | 39:YT:67:SER:HB2   | 2.00                     | 0.43              |
| 5:QE:35:GLY:HA3    | 5:QE:112:LEU:HB3   | 1.99                     | 0.43              |
| 1:XA:524:G:H2'     | 1:XA:525:C:C6      | 2.53                     | 0.43              |
| 17:QQ:58:GLU:O     | 17:QQ:74:LEU:N     | 2.50                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:1712:C:H2'  | 25:RA:1713:U:H6    | 1.83                     | 0.43              |
| 25:RA:1441:G:O2'  | 25:RA:1442:G:H5'   | 2.19                     | 0.43              |
| 54:R8:22:VAL:HB   | 54:R8:50:LEU:HD12  | 2.00                     | 0.43              |
| 20:XT:23:ARG:O    | 20:XT:27:LYS:HB2   | 2.18                     | 0.43              |
| 1:QA:1014:A:C2    | 1:QA:1219:U:H1'    | 2.54                     | 0.43              |
| 1:QA:490:G:H2'    | 1:QA:491:G:H8      | 1.84                     | 0.43              |
| 25:YA:1648:C:H2'  | 25:YA:1649:G:O4'   | 2.18                     | 0.43              |
| 24:QY:76:PHE:HB3  | 24:QY:86:LEU:HD13  | 1.99                     | 0.43              |
| 25:YA:2394:C:OP1  | 35:YP:63:PRO:HD2   | 2.19                     | 0.43              |
| 47:Y1:84:GLY:O    | 47:Y1:87:PRO:HD2   | 2.19                     | 0.43              |
| 31:YH:7:LEU:HD13  | 31:YH:69:ARG:HB3   | 1.99                     | 0.43              |
| 25:YA:607:U:H3    | 25:YA:621:A:H2     | 1.61                     | 0.43              |
| 25:RA:9:U:H5'     | 33:RN:115:ARG:HH12 | 1.84                     | 0.43              |
| 25:YA:335:C:H4'   | 44:YY:73:ARG:HD2   | 2.00                     | 0.43              |
| 27:RD:35:LYS:HB3  | 27:RD:63:ARG:HA    | 2.01                     | 0.43              |
| 25:RA:1186:G:H2'  | 25:RA:1187:G:O4'   | 2.18                     | 0.43              |
| 37:YR:38:VAL:HB   | 37:YR:39:PRO:HD3   | 2.00                     | 0.43              |
| 25:RA:2660:A:H2'  | 25:RA:2661:G:O4'   | 2.19                     | 0.43              |
| 2:XB:17:PHE:CD2   | 2:XB:41:ILE:HG23   | 2.54                     | 0.43              |
| 1:XA:1219:U:P     | 14:XN:19:ARG:HH12  | 2.40                     | 0.43              |
| 25:YA:489:G:H2'   | 25:YA:491:G:O4'    | 2.19                     | 0.43              |
| 25:YA:394:A:N6    | 25:YA:395:U:O4     | 2.52                     | 0.43              |
| 1:XA:637:G:H2'    | 1:XA:638:G:C8      | 2.54                     | 0.43              |
| 25:YA:2557:G:H2'  | 25:YA:2558:C:C6    | 2.54                     | 0.43              |
| 46:Y0:40:GLN:OE1  | 46:Y0:44:ARG:N     | 2.51                     | 0.43              |
| 1:QA:790:A:OP1    | 22:QV:38:A:O2'     | 2.28                     | 0.43              |
| 12:XL:58:VAL:O    | 12:XL:65:GLU:HA    | 2.18                     | 0.43              |
| 1:QA:429:U:H1'    | 1:QA:430:A:H5''    | 2.00                     | 0.43              |
| 24:QY:46:LEU:O    | 24:QY:53:LEU:HD22  | 2.18                     | 0.43              |
| 25:YA:1973:G:H2'  | 25:YA:1974:C:C6    | 2.54                     | 0.43              |
| 25:RA:1345:C:H2'  | 25:RA:1346:G:H8    | 1.84                     | 0.43              |
| 53:R7:47:ARG:H    | 53:R7:47:ARG:HH11  | 1.66                     | 0.43              |
| 13:QM:16:ASP:N    | 13:QM:16:ASP:OD2   | 2.50                     | 0.43              |
| 37:RR:103:ARG:HD3 | 37:RR:103:ARG:HA   | 1.82                     | 0.43              |
| 5:XE:5:ASP:N      | 5:XE:5:ASP:OD1     | 2.52                     | 0.43              |
| 25:YA:2281:C:O2'  | 25:YA:2282:G:H5'   | 2.19                     | 0.43              |
| 41:RV:89:GLN:HA   | 41:RV:90:PRO:HD3   | 1.89                     | 0.43              |
| 4:QD:171:GLY:HA2  | 4:QD:172:PRO:HD3   | 1.87                     | 0.43              |
| 25:YA:922:U:H1'   | 46:Y0:26:TYR:CD1   | 2.54                     | 0.43              |
| 1:QA:966:G:C2     | 22:QV:34:C:H5'     | 2.54                     | 0.43              |
| 7:QG:86:GLN:CD    | 22:QW:31:G:H21     | 2.19                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:1576:U:H2'  | 25:RA:1577:C:H6    | 1.84                     | 0.43              |
| 44:RY:19:LYS:HE3  | 44:RY:71:LYS:HZ1   | 1.83                     | 0.43              |
| 19:XS:36:ARG:HH12 | 19:XS:73:GLU:HB2   | 1.82                     | 0.43              |
| 1:QA:717:C:H4'    | 11:QK:117:ASN:HB2  | 2.01                     | 0.43              |
| 52:R6:40:CYS:HB3  | 52:R6:46:HIS:CG    | 2.53                     | 0.43              |
| 39:YT:102:ILE:O   | 39:YT:106:SER:HB3  | 2.19                     | 0.43              |
| 36:RQ:81:VAL:HG23 | 46:R0:7:LEU:HD11   | 2.00                     | 0.43              |
| 3:QC:22:TRP:CD1   | 3:QC:59:ARG:HD2    | 2.53                     | 0.43              |
| 9:XI:37:PHE:CE2   | 9:XI:70:LYS:HG3    | 2.54                     | 0.43              |
| 25:YA:676:A:H1'   | 25:YA:2443:C:H1'   | 2.01                     | 0.43              |
| 36:YQ:63:LYS:HD2  | 45:YZ:175:VAL:HG21 | 2.01                     | 0.43              |
| 25:RA:1668:A:H5'' | 34:RO:5:GLN:HG2    | 2.01                     | 0.43              |
| 1:XA:445:G:H2'    | 1:XA:446:G:C8      | 2.53                     | 0.43              |
| 25:YA:1357:U:H4'  | 53:Y7:23:ARG:HH21  | 1.84                     | 0.43              |
| 30:RG:143:GLU:HG2 | 50:R4:26:SER:HB2   | 2.01                     | 0.43              |
| 25:YA:862:G:O2'   | 26:YB:78:A:N3      | 2.48                     | 0.43              |
| 25:RA:484:C:H2'   | 25:RA:485:C:C6     | 2.54                     | 0.43              |
| 34:YO:104:ARG:HG2 | 34:YO:121:VAL:HG12 | 2.01                     | 0.43              |
| 1:QA:1218:C:H2'   | 1:QA:1219:U:C6     | 2.53                     | 0.43              |
| 20:XT:58:LYS:HE2  | 20:XT:62:LEU:HD21  | 2.00                     | 0.43              |
| 39:YT:6:LEU:O     | 39:YT:10:VAL:HG23  | 2.19                     | 0.43              |
| 44:RY:11:ASP:O    | 44:RY:27:VAL:HG23  | 2.19                     | 0.43              |
| 33:RN:12:ARG:O    | 33:RN:50:ASP:HB2   | 2.18                     | 0.43              |
| 25:YA:2741:A:H2'  | 25:YA:2742:C:O4'   | 2.19                     | 0.43              |
| 25:YA:1500:G:H21  | 27:YD:100:GLY:HA3  | 1.83                     | 0.43              |
| 25:RA:1060:U:H3   | 25:RA:1088:A:H8    | 1.66                     | 0.43              |
| 1:XA:1163:C:H2'   | 1:XA:1164:G:C8     | 2.53                     | 0.43              |
| 38:RS:19:LYS:O    | 38:RS:21:THR:N     | 2.50                     | 0.43              |
| 30:RG:112:PRO:HG2 | 50:R4:37:SER:CB    | 2.49                     | 0.43              |
| 19:XS:32:LYS:HB2  | 19:XS:32:LYS:HE2   | 1.60                     | 0.43              |
| 21:XU:15:ARG:HD3  | 21:XU:15:ARG:HA    | 1.82                     | 0.43              |
| 1:QA:939:G:H5''   | 7:QG:102:ARG:NH2   | 2.34                     | 0.43              |
| 36:RQ:65:PHE:O    | 36:RQ:104:PHE:HA   | 2.19                     | 0.43              |
| 43:YX:25:LYS:NZ   | 43:YX:82:GLN:OE1   | 2.51                     | 0.43              |
| 1:QA:304:U:H2'    | 1:QA:305:G:C8      | 2.53                     | 0.43              |
| 1:QA:1121:U:H2'   | 1:QA:1122:U:C6     | 2.54                     | 0.43              |
| 28:RE:12:THR:HB   | 28:RE:13:ARG:H     | 1.59                     | 0.43              |
| 13:XM:10:PRO:HD2  | 13:XM:18:ALA:HB1   | 2.00                     | 0.43              |
| 25:RA:1912:A:C2'  | 25:RA:1913:A:O5'   | 2.67                     | 0.43              |
| 23:QX:13:A:O2'    | 23:QX:14:A:H3'     | 2.18                     | 0.43              |
| 1:XA:530:G:H2'    | 24:XY:70:ALA:HA    | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:RH:42:ARG:HD2  | 31:RH:42:ARG:HA   | 1.78                     | 0.43              |
| 10:QJ:4:ILE:HB    | 10:QJ:74:ILE:HG12 | 2.01                     | 0.43              |
| 13:QM:4:ILE:HG23  | 13:QM:5:ALA:H     | 1.82                     | 0.43              |
| 25:RA:1264:G:H3'  | 25:RA:1265:A:H5'' | 2.00                     | 0.43              |
| 25:YA:2481:G:HO2' | 25:YA:2482:G:P    | 2.42                     | 0.43              |
| 25:RA:1374:G:H2'  | 25:RA:1375:C:H6   | 1.84                     | 0.43              |
| 1:QA:1033:G:HO2'  | 1:QA:1034:G:P     | 2.39                     | 0.43              |
| 8:QH:37:ARG:O     | 8:QH:41:ARG:HB2   | 2.19                     | 0.43              |
| 20:QT:55:ILE:HA   | 20:QT:55:ILE:HD13 | 1.87                     | 0.43              |
| 25:RA:2695:C:H2'  | 25:RA:2696:U:C6   | 2.53                     | 0.43              |
| 25:RA:300:A:H1'   | 25:RA:319:C:H1'   | 2.01                     | 0.43              |
| 30:YG:10:LYS:HE2  | 30:YG:175:LEU:O   | 2.19                     | 0.43              |
| 25:RA:1798:U:H5'  | 27:RD:259:THR:HG1 | 1.83                     | 0.43              |
| 40:RU:8:VAL:HG12  | 40:RU:11:ARG:NH2  | 2.34                     | 0.43              |
| 25:YA:821:A:H2'   | 25:YA:946:G:H5''  | 2.00                     | 0.43              |
| 1:XA:1140:C:H2'   | 1:XA:1141:C:C6    | 2.54                     | 0.43              |
| 1:QA:833:U:H2'    | 1:QA:834:C:H6     | 1.84                     | 0.43              |
| 28:YE:3:GLY:HA2   | 28:YE:198:VAL:O   | 2.18                     | 0.43              |
| 1:QA:885:G:OP2    | 1:QA:885:G:H8     | 2.00                     | 0.43              |
| 29:RF:117:ARG:HD3 | 29:RF:117:ARG:HA  | 1.57                     | 0.43              |
| 34:RO:87:ILE:CG2  | 34:RO:91:LEU:HA   | 2.49                     | 0.43              |
| 1:QA:108:G:N2     | 20:QT:12:ALA:HB1  | 2.34                     | 0.43              |
| 8:XH:121:ASP:OD2  | 8:XH:122:ARG:HG3  | 2.19                     | 0.43              |
| 25:YA:738:G:H3'   | 25:YA:739:G:C8    | 2.54                     | 0.43              |
| 27:RD:24:ILE:HD11 | 27:RD:84:TYR:HB2  | 2.01                     | 0.43              |
| 25:YA:999:U:H2'   | 25:YA:1000:A:H5'' | 2.01                     | 0.43              |
| 25:RA:2785:C:O2'  | 28:RE:64:LYS:HD3  | 2.19                     | 0.43              |
| 40:RU:50:ARG:O    | 40:RU:54:LYS:NZ   | 2.40                     | 0.43              |
| 1:QA:1347:G:N7    | 9:QI:107:ARG:HB3  | 2.34                     | 0.43              |
| 40:RU:92:ARG:NH2  | 41:RV:11:GLN:HG3  | 2.34                     | 0.43              |
| 50:R4:55:ARG:NE   | 50:R4:55:ARG:H    | 2.17                     | 0.43              |
| 2:QB:7:VAL:HG13   | 2:QB:8:LYS:H      | 1.84                     | 0.43              |
| 25:YA:2645:G:H3'  | 25:YA:2646:C:C5'  | 2.49                     | 0.43              |
| 1:XA:1318:A:O2'   | 19:XS:37:ARG:HG2  | 2.19                     | 0.43              |
| 21:QU:9:ARG:O     | 21:QU:13:ILE:HG13 | 2.19                     | 0.43              |
| 11:XK:98:LEU:HA   | 11:XK:98:LEU:HD23 | 1.87                     | 0.43              |
| 25:RA:2666:C:N3   | 31:RH:152:ARG:NH2 | 2.67                     | 0.43              |
| 42:YW:18:ARG:NH1  | 42:YW:76:VAL:O    | 2.52                     | 0.43              |
| 25:YA:2838:G:O2'  | 37:YR:45:ARG:NH1  | 2.52                     | 0.43              |
| 28:YE:23:VAL:HA   | 28:YE:184:VAL:O   | 2.19                     | 0.43              |
| 31:YH:33:LEU:HA   | 31:YH:33:LEU:HD12 | 1.78                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:QP:5:ARG:NH2   | 16:QP:24:ALA:HA   | 2.34                     | 0.43              |
| 1:QA:1137:C:H5'   | 1:QA:1138:G:C2    | 2.53                     | 0.43              |
| 25:RA:2811:G:H8   | 25:RA:2811:G:OP2  | 2.02                     | 0.43              |
| 1:QA:1429:C:H2'   | 1:QA:1430:C:C6    | 2.53                     | 0.43              |
| 1:XA:443:C:H2'    | 1:XA:444:C:C6     | 2.54                     | 0.43              |
| 16:QP:11:SER:HB2  | 16:QP:14:ASN:HB3  | 2.01                     | 0.43              |
| 25:YA:2130:U:O2   | 25:YA:2133:G:O2'  | 2.36                     | 0.43              |
| 50:R4:14:ILE:O    | 50:R4:21:VAL:HG23 | 2.19                     | 0.43              |
| 25:RA:2078:C:H1'  | 25:RA:2434:A:N3   | 2.34                     | 0.43              |
| 9:XI:18:PHE:HB2   | 9:XI:62:TYR:HB3   | 2.01                     | 0.43              |
| 25:RA:324:A:N6    | 25:RA:338:G:O2'   | 2.50                     | 0.43              |
| 10:QJ:33:GLN:H    | 10:QJ:75:ILE:HG12 | 1.84                     | 0.43              |
| 36:RQ:2:LEU:HD12  | 36:RQ:2:LEU:H     | 1.83                     | 0.43              |
| 9:QI:128:ARG:NH2  | 22:QV:33:U:OP2    | 2.52                     | 0.43              |
| 25:RA:2467:C:H4'  | 36:RQ:123:HIS:CD2 | 2.54                     | 0.43              |
| 1:XA:662:G:H2'    | 1:XA:663:A:C8     | 2.54                     | 0.43              |
| 25:RA:1105:U:H2'  | 25:RA:1106:G:H8   | 1.83                     | 0.43              |
| 32:YI:128:LEU:O   | 32:YI:138:ILE:N   | 2.52                     | 0.42              |
| 25:RA:2786:U:H5'' | 28:RE:66:HIS:CD2  | 2.54                     | 0.42              |
| 25:YA:2543:G:H21  | 25:YA:2646:C:H5'' | 1.83                     | 0.42              |
| 1:XA:1179:A:H4'   | 9:XI:103:THR:HA   | 2.00                     | 0.42              |
| 10:QJ:8:LEU:HD22  | 10:QJ:20:ALA:HB2  | 1.99                     | 0.42              |
| 39:RT:26:ASP:HB3  | 39:RT:92:GLY:H    | 1.83                     | 0.42              |
| 25:RA:2496:C:OP1  | 36:RQ:81:VAL:HG12 | 2.18                     | 0.42              |
| 1:XA:1029:C:H2'   | 1:XA:1030:C:C6    | 2.54                     | 0.42              |
| 25:RA:1503:U:H2'  | 25:RA:1504:C:C6   | 2.53                     | 0.42              |
| 25:RA:859:G:H1'   | 25:RA:860:U:H5    | 1.83                     | 0.42              |
| 26:YB:114:G:O4'   | 38:YS:47:THR:HB   | 2.19                     | 0.42              |
| 40:YU:98:LEU:O    | 40:YU:99:ALA:HB3  | 2.19                     | 0.42              |
| 25:YA:1278:A:H2'  | 25:YA:1279:G:C8   | 2.54                     | 0.42              |
| 25:YA:2516:G:C6   | 25:YA:2517:C:N4   | 2.87                     | 0.42              |
| 3:XC:179:ARG:HH11 | 3:XC:207:VAL:HG22 | 1.84                     | 0.42              |
| 1:XA:500:G:N2     | 1:XA:546:G:H1'    | 2.33                     | 0.42              |
| 25:YA:1666:G:H2'  | 25:YA:1667:G:H1'  | 2.00                     | 0.42              |
| 25:RA:1036:G:H2'  | 25:RA:1037:G:O4'  | 2.18                     | 0.42              |
| 1:XA:131:C:H2'    | 1:XA:132:C:C6     | 2.53                     | 0.42              |
| 10:XJ:6:ILE:HG22  | 10:XJ:98:ILE:HA   | 2.00                     | 0.42              |
| 29:RF:32:LEU:O    | 29:RF:36:VAL:HG23 | 2.19                     | 0.42              |
| 2:XB:133:LYS:HD2  | 2:XB:137:ARG:NH1  | 2.34                     | 0.42              |
| 7:QG:46:ALA:O     | 7:QG:50:ILE:HG12  | 2.19                     | 0.42              |
| 25:RA:2817:G:OP1  | 37:RR:99:LYS:HE2  | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:XA:281:G:OP2     | 1:XA:281:G:H8      | 2.01                     | 0.42              |
| 25:RA:1429:G:H2'   | 25:RA:1430:C:C6    | 2.54                     | 0.42              |
| 1:QA:16:A:N1       | 1:QA:919:A:H2      | 2.17                     | 0.42              |
| 51:Y5:9:LYS:HA     | 51:Y5:9:LYS:HD3    | 1.86                     | 0.42              |
| 12:XL:46:LYS:HB3   | 12:XL:46:LYS:HE2   | 1.81                     | 0.42              |
| 55:R9:32:HIS:O     | 55:R9:34:GLN:HG3   | 2.19                     | 0.42              |
| 1:XA:922:G:C6      | 1:XA:923:A:C6      | 3.06                     | 0.42              |
| 25:RA:2102:U:H2'   | 25:RA:2103:C:C6    | 2.53                     | 0.42              |
| 25:YA:2589:A:H2'   | 25:YA:2590:A:C8    | 2.54                     | 0.42              |
| 47:R1:34:THR:HG22  | 47:R1:36:GLY:H     | 1.84                     | 0.42              |
| 47:Y1:86:SER:N     | 47:Y1:87:PRO:HD2   | 2.34                     | 0.42              |
| 1:QA:664:G:P       | 18:QR:64:ARG:HH21  | 2.42                     | 0.42              |
| 38:RS:62:LYS:HD3   | 38:RS:97:ARG:NH1   | 2.35                     | 0.42              |
| 25:YA:1006:C:C2    | 25:YA:1138:G:N2    | 2.87                     | 0.42              |
| 3:QC:19:GLU:HG2    | 3:QC:40:ARG:NH2    | 2.34                     | 0.42              |
| 35:YP:146:VAL:HG13 | 35:YP:147:LEU:HD22 | 2.01                     | 0.42              |
| 50:Y4:60:GLN:HB3   | 50:Y4:61:ARG:NH2   | 2.34                     | 0.42              |
| 7:XG:20:ASP:O      | 7:XG:21:VAL:HG22   | 2.19                     | 0.42              |
| 25:RA:1675:C:O2    | 28:RE:128:SER:OG   | 2.37                     | 0.42              |
| 10:XJ:56:HIS:O     | 10:XJ:57:LYS:C     | 2.57                     | 0.42              |
| 25:RA:878:A:H3'    | 25:RA:879:G:H8     | 1.84                     | 0.42              |
| 4:QD:92:VAL:O      | 4:QD:96:LEU:HD22   | 2.19                     | 0.42              |
| 25:RA:248:G:H5'    | 25:RA:250:G:N7     | 2.34                     | 0.42              |
| 25:RA:2314:C:C5'   | 30:RG:38:VAL:HG11  | 2.49                     | 0.42              |
| 30:YG:7:LEU:HB2    | 30:YG:104:GLU:OE1  | 2.18                     | 0.42              |
| 40:YU:100:VAL:C    | 40:YU:102:GLU:H    | 2.22                     | 0.42              |
| 22:XW:65:C:H2'     | 22:XW:66:C:C6      | 2.54                     | 0.42              |
| 1:QA:56:U:H2'      | 1:QA:57:G:H8       | 1.84                     | 0.42              |
| 30:RG:99:MET:HG3   | 30:RG:100:TRP:N    | 2.34                     | 0.42              |
| 1:QA:1256:A:H1'    | 1:QA:1258:G:C6     | 2.54                     | 0.42              |
| 1:XA:1427:U:H2'    | 1:XA:1428:A:C8     | 2.53                     | 0.42              |
| 25:RA:444:C:H4'    | 29:RF:49:ALA:HB2   | 2.01                     | 0.42              |
| 12:QL:39:VAL:HG12  | 12:QL:41:ARG:HG3   | 2.01                     | 0.42              |
| 1:XA:1277:C:O2'    | 1:XA:1279:A:H8     | 2.02                     | 0.42              |
| 25:RA:1805:U:O2    | 27:RD:50:THR:HB    | 2.19                     | 0.42              |
| 1:XA:1206:G:C6     | 1:XA:1207:G:C5     | 3.07                     | 0.42              |
| 25:RA:862:G:H2'    | 25:RA:863:A:O4'    | 2.19                     | 0.42              |
| 48:R2:53:LEU:O     | 48:R2:56:GLN:HB2   | 2.18                     | 0.42              |
| 25:YA:1313:U:H2'   | 25:YA:1610:A:C2    | 2.54                     | 0.42              |
| 5:XE:69:VAL:HA     | 5:XE:70:PRO:HD2    | 1.90                     | 0.42              |
| 42:YW:9:TYR:H      | 42:YW:102:HIS:CE1  | 2.37                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:YD:108:PRO:HB3 | 27:YD:143:HIS:NE2 | 2.34                     | 0.42              |
| 25:YA:2676:C:OP1  | 34:YO:31:LYS:NZ   | 2.51                     | 0.42              |
| 1:QA:923:A:OP1    | 5:QE:21:ALA:HB2   | 2.19                     | 0.42              |
| 1:XA:1010:G:H1    | 1:XA:1019:C:H42   | 1.66                     | 0.42              |
| 25:RA:1939:U:OP1  | 25:RA:2604:U:O2'  | 2.30                     | 0.42              |
| 25:YA:649:G:H2'   | 25:YA:650:C:C6    | 2.55                     | 0.42              |
| 13:XM:18:ALA:HB2  | 13:XM:45:VAL:HG21 | 2.01                     | 0.42              |
| 45:RZ:59:LEU:HD21 | 45:RZ:67:LEU:HB2  | 2.01                     | 0.42              |
| 25:YA:2633:G:H1'  | 28:YE:62:PRO:CB   | 2.50                     | 0.42              |
| 25:RA:993:G:H1'   | 41:RV:87:HIS:CE1  | 2.54                     | 0.42              |
| 41:YV:70:ILE:HG13 | 41:YV:86:GLY:O    | 2.19                     | 0.42              |
| 41:YV:85:LYS:CG   | 41:YV:87:HIS:H    | 2.24                     | 0.42              |
| 40:RU:92:ARG:HH22 | 41:RV:11:GLN:H    | 1.67                     | 0.42              |
| 29:YF:25:PRO:HB3  | 29:YF:28:ILE:HG12 | 2.01                     | 0.42              |
| 20:XT:67:ALA:HA   | 20:XT:73:HIS:N    | 2.30                     | 0.42              |
| 25:YA:1049:C:O2   | 25:YA:1113:U:O2'  | 2.30                     | 0.42              |
| 25:RA:2343:C:C5'  | 25:RA:2343:C:C6   | 2.96                     | 0.42              |
| 39:RT:91:ARG:HD2  | 39:RT:124:ASP:OD2 | 2.18                     | 0.42              |
| 25:YA:2477:C:H1'  | 25:YA:2481:G:O6   | 2.18                     | 0.42              |
| 1:XA:267:C:P      | 17:XQ:67:LYS:HB2  | 2.59                     | 0.42              |
| 4:QD:96:LEU:HD12  | 4:QD:139:ARG:NH1  | 2.34                     | 0.42              |
| 25:RA:1028:A:N6   | 25:RA:1125:G:H2'  | 2.34                     | 0.42              |
| 25:YA:2336:A:H61  | 46:Y0:43:THR:CG2  | 2.32                     | 0.42              |
| 1:QA:781:A:H4'    | 1:QA:1522:U:O2'   | 2.18                     | 0.42              |
| 34:RO:34:THR:OG1  | 34:RO:35:VAL:N    | 2.52                     | 0.42              |
| 34:YO:15:GLY:O    | 34:YO:47:ILE:N    | 2.47                     | 0.42              |
| 25:YA:2328:A:H2'  | 25:YA:2329:G:C8   | 2.55                     | 0.42              |
| 29:RF:164:ARG:HG3 | 29:RF:175:THR:OG1 | 2.19                     | 0.42              |
| 25:RA:871:U:OP1   | 36:RQ:5:ARG:N     | 2.51                     | 0.42              |
| 25:RA:1796:U:H2'  | 25:RA:1797:C:H6   | 1.85                     | 0.42              |
| 25:RA:1423:G:H2'  | 25:RA:1424:G:H8   | 1.84                     | 0.42              |
| 25:RA:2364:C:H2'  | 25:RA:2365:G:O4'  | 2.20                     | 0.42              |
| 29:RF:103:LYS:HG2 | 29:RF:106:ARG:NH2 | 2.34                     | 0.42              |
| 40:YU:83:LEU:HG   | 40:YU:88:ILE:HD11 | 2.01                     | 0.42              |
| 25:RA:2115:G:N7   | 25:RA:2117:A:H5'' | 2.33                     | 0.42              |
| 25:YA:2577:A:H5'' | 25:YA:2578:G:H5'  | 2.00                     | 0.42              |
| 46:Y0:24:LYS:C    | 46:Y0:25:ARG:HD2  | 2.40                     | 0.42              |
| 1:XA:1159:U:O2'   | 1:XA:1160:G:N7    | 2.53                     | 0.42              |
| 44:YY:96:ILE:HD12 | 44:YY:98:VAL:HG12 | 2.00                     | 0.42              |
| 35:RP:14:LYS:C    | 35:RP:16:ARG:N    | 2.73                     | 0.42              |
| 25:RA:910:A:N1    | 25:RA:2277:G:H1'  | 2.34                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:YD:92:ILE:HD12 | 27:YD:104:TYR:CD2  | 2.54                     | 0.42              |
| 1:QA:316:G:O5'    | 1:QA:316:G:C8      | 2.72                     | 0.42              |
| 1:XA:518:C:H2'    | 1:XA:530:G:C8      | 2.54                     | 0.42              |
| 9:QI:16:ARG:O     | 9:QI:63:ILE:HA     | 2.18                     | 0.42              |
| 25:YA:569:U:C4    | 25:YA:570:G:C6     | 3.07                     | 0.42              |
| 21:XU:9:ARG:O     | 21:XU:13:ILE:HG13  | 2.19                     | 0.42              |
| 33:YN:34:LEU:HD22 | 33:YN:119:ARG:HB2  | 2.00                     | 0.42              |
| 25:RA:2199:A:C5   | 25:RA:2225:A:C6    | 3.08                     | 0.42              |
| 1:XA:1314:C:OP2   | 19:XS:6:LYS:HD2    | 2.19                     | 0.42              |
| 36:YQ:77:LYS:HG3  | 36:YQ:86:GLY:HA2   | 2.02                     | 0.42              |
| 1:XA:1030:C:H3'   | 1:XA:1030(A):G:H4' | 2.00                     | 0.42              |
| 35:RP:86:LYS:HB3  | 35:RP:117:GLU:O    | 2.19                     | 0.42              |
| 30:RG:11:TYR:HA   | 30:RG:15:VAL:HB    | 2.00                     | 0.42              |
| 1:QA:1059:C:O2'   | 10:QJ:53:PRO:HD3   | 2.19                     | 0.42              |
| 25:RA:1963:U:H3'  | 25:RA:1963:U:O2    | 2.19                     | 0.42              |
| 50:Y4:9:LEU:HD23  | 50:Y4:25:TYR:HB3   | 2.01                     | 0.42              |
| 25:YA:1169:G:H1   | 25:YA:1180:C:H42   | 1.68                     | 0.42              |
| 25:RA:569:U:C4    | 25:RA:570:G:C6     | 3.07                     | 0.42              |
| 1:QA:1277:C:O2'   | 1:QA:1279:A:H1'    | 2.19                     | 0.42              |
| 25:YA:909:A:H2'   | 25:YA:912:C:H5     | 1.83                     | 0.42              |
| 1:QA:834:C:C4     | 1:QA:835:U:C4      | 3.07                     | 0.42              |
| 2:XB:102:LEU:HD23 | 2:XB:182:ILE:HD12  | 2.02                     | 0.42              |
| 3:XC:34:LEU:HD13  | 14:XN:25:VAL:HG11  | 2.00                     | 0.42              |
| 3:XC:8:ILE:HG23   | 3:XC:16:ARG:HG2    | 2.01                     | 0.42              |
| 1:QA:881:G:OP2    | 12:QL:12:ARG:NH2   | 2.51                     | 0.42              |
| 19:XS:79:THR:O    | 19:XS:81:ARG:N     | 2.52                     | 0.42              |
| 13:XM:54:VAL:HG22 | 13:XM:57:ARG:NH2   | 2.34                     | 0.42              |
| 25:YA:1036:G:OP1  | 31:YH:59:ARG:HB2   | 2.19                     | 0.42              |
| 1:XA:236:G:OP1    | 17:XQ:40:LYS:NZ    | 2.49                     | 0.42              |
| 48:Y2:50:ILE:HD12 | 48:Y2:51:ARG:H     | 1.85                     | 0.42              |
| 25:RA:2376:A:H2'  | 25:RA:2377:A:O4'   | 2.19                     | 0.42              |
| 28:YE:97:LYS:N    | 28:YE:100:GLU:OE1  | 2.48                     | 0.42              |
| 1:QA:272:C:H2'    | 1:QA:273:A:H8      | 1.85                     | 0.42              |
| 1:QA:1369:C:H2'   | 1:QA:1370:G:C8     | 2.55                     | 0.42              |
| 11:XK:124:LYS:HE2 | 11:XK:124:LYS:HB3  | 1.71                     | 0.42              |
| 16:XP:54:GLU:H    | 16:XP:54:GLU:CD    | 2.23                     | 0.42              |
| 25:YA:1441:G:O2'  | 25:YA:1628:G:OP1   | 2.33                     | 0.42              |
| 25:YA:2022:U:O2'  | 25:YA:2617:C:H5'   | 2.19                     | 0.42              |
| 22:XV:25:C:H2'    | 22:XV:26:G:O4'     | 2.19                     | 0.42              |
| 1:QA:1490:C:H2'   | 1:QA:1491:G:O5'    | 2.17                     | 0.42              |
| 25:YA:1912:A:O2'  | 25:YA:1913:A:OP1   | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:6:A:C4      | 25:YA:7:G:C8      | 3.07                     | 0.42              |
| 1:QA:1391:U:H2'   | 1:QA:1392:G:C8    | 2.54                     | 0.42              |
| 2:QB:186:ALA:O    | 2:QB:201:ILE:N    | 2.50                     | 0.42              |
| 41:RV:71:LEU:HD12 | 41:RV:71:LEU:HA   | 1.64                     | 0.42              |
| 5:QE:127:ASN:HA   | 5:QE:128:PRO:HD3  | 1.85                     | 0.42              |
| 25:RA:1911:U:H2'  | 25:RA:1918:A:C2   | 2.54                     | 0.42              |
| 1:QA:485:G:HO2'   | 1:QA:486:U:P      | 2.42                     | 0.42              |
| 35:YP:39:LYS:HB2  | 35:YP:45:LEU:HD23 | 2.00                     | 0.42              |
| 44:RY:42:VAL:O    | 44:RY:65:ALA:N    | 2.38                     | 0.42              |
| 7:XG:20:ASP:CG    | 7:XG:23:VAL:HB    | 2.39                     | 0.42              |
| 35:YP:101:VAL:HA  | 35:YP:105:LEU:O   | 2.20                     | 0.42              |
| 1:QA:738:C:H2'    | 1:QA:739:C:H6     | 1.85                     | 0.42              |
| 22:QV:12:G:H4'    | 25:RA:1908:C:O2   | 2.19                     | 0.42              |
| 28:YE:144:ARG:HB3 | 28:YE:145:LYS:H   | 1.42                     | 0.42              |
| 14:QN:6:LEU:HD22  | 14:QN:23:ARG:HH22 | 1.83                     | 0.42              |
| 25:YA:2838:G:C1'  | 37:YR:45:ARG:HH12 | 2.32                     | 0.42              |
| 27:YD:97:TYR:CB   | 27:YD:99:ASP:OD1  | 2.67                     | 0.42              |
| 40:YU:58:ARG:HA   | 40:YU:61:TRP:CE3  | 2.54                     | 0.42              |
| 1:QA:277:C:H2'    | 1:QA:278:G:C8     | 2.54                     | 0.42              |
| 25:YA:1265:A:H8   | 25:YA:1265:A:OP1  | 2.02                     | 0.42              |
| 1:QA:1513:A:H2'   | 1:QA:1514:C:C6    | 2.54                     | 0.42              |
| 1:XA:1388:C:H2'   | 1:XA:1389:C:C6    | 2.55                     | 0.42              |
| 25:RA:389:G:H1    | 35:RP:71:VAL:HG12 | 1.83                     | 0.42              |
| 1:XA:637:G:H2'    | 1:XA:638:G:H8     | 1.85                     | 0.42              |
| 25:RA:2645:G:H3'  | 25:RA:2646:C:H5'  | 2.01                     | 0.42              |
| 25:YA:2040:C:H2'  | 25:YA:2041:U:C6   | 2.55                     | 0.42              |
| 25:YA:26:G:C6     | 25:YA:27:G:N1     | 2.88                     | 0.42              |
| 22:QW:28:C:H42    | 22:QW:42:G:H1     | 1.67                     | 0.42              |
| 12:QL:102:ARG:HB3 | 12:QL:102:ARG:HE  | 1.67                     | 0.42              |
| 25:RA:2389:G:H5'' | 25:RA:2390:U:O4'  | 2.19                     | 0.42              |
| 20:XT:58:LYS:O    | 20:XT:58:LYS:HD3  | 2.19                     | 0.42              |
| 25:RA:862:G:O2'   | 26:RB:78:A:N3     | 2.50                     | 0.42              |
| 17:XQ:95:TYR:O    | 17:XQ:98:LEU:N    | 2.52                     | 0.42              |
| 36:RQ:43:THR:HG22 | 36:RQ:94:VAL:HG12 | 2.00                     | 0.42              |
| 7:XG:14:PRO:HB2   | 7:XG:19:GLY:HA2   | 2.01                     | 0.42              |
| 43:YX:14:SER:H    | 43:YX:17:ALA:HB3  | 1.84                     | 0.42              |
| 1:XA:538:G:H5''   | 12:XL:114:LYS:HB2 | 2.01                     | 0.42              |
| 1:QA:892:A:O2'    | 1:QA:1415:G:H4'   | 2.19                     | 0.42              |
| 25:RA:1239:G:H2'  | 25:RA:1240:U:O4'  | 2.19                     | 0.42              |
| 5:QE:82:VAL:HG21  | 5:QE:138:ALA:HA   | 2.02                     | 0.42              |
| 1:QA:1182:G:O2'   | 1:QA:1183:A:OP2   | 2.35                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:XH:1:MET:SD      | 8:XH:1:MET:N       | 2.77                     | 0.42              |
| 42:YW:82:LEU:HA    | 42:YW:82:LEU:HD23  | 1.89                     | 0.42              |
| 48:R2:28:LYS:HA    | 48:R2:28:LYS:HD3   | 1.88                     | 0.42              |
| 45:RZ:139:VAL:HG13 | 45:RZ:139:VAL:O    | 2.19                     | 0.42              |
| 41:RV:68:LYS:HD3   | 41:RV:68:LYS:HA    | 1.87                     | 0.42              |
| 36:YQ:60:ARG:O     | 45:YZ:177:PRO:HB2  | 2.19                     | 0.42              |
| 37:YR:104:ARG:HB3  | 37:YR:107:ASP:OD2  | 2.19                     | 0.42              |
| 8:XH:86:ILE:HG12   | 8:XH:135:CYS:HA    | 2.01                     | 0.42              |
| 44:YY:101:LYS:O    | 44:YY:101:LYS:HE3  | 2.20                     | 0.42              |
| 52:R6:18:ARG:HG3   | 52:R6:44:ARG:NH1   | 2.34                     | 0.42              |
| 46:Y0:7:LEU:HD13   | 46:Y0:7:LEU:HA     | 1.93                     | 0.42              |
| 25:RA:2208:A:N3    | 25:RA:2219:G:N2    | 2.67                     | 0.42              |
| 2:XB:200:ILE:HG22  | 2:XB:202:PRO:HD3   | 2.02                     | 0.42              |
| 25:RA:129:C:H2'    | 25:RA:130:C:C6     | 2.55                     | 0.42              |
| 25:RA:1414:G:H1    | 25:RA:1588:C:H42   | 1.68                     | 0.42              |
| 44:RY:65:ALA:HA    | 44:RY:66:PRO:HD3   | 1.90                     | 0.42              |
| 25:YA:2579:C:C4'   | 28:YE:134:ILE:HG21 | 2.49                     | 0.42              |
| 28:RE:23:VAL:O     | 28:RE:24:THR:OG1   | 2.22                     | 0.42              |
| 1:QA:921:U:O2'     | 5:QE:18:ARG:O      | 2.37                     | 0.42              |
| 2:QB:69:LEU:HA     | 2:QB:91:PRO:HG2    | 2.01                     | 0.42              |
| 41:YV:21:ARG:HG2   | 41:YV:93:GLU:HG3   | 2.01                     | 0.42              |
| 25:RA:1952:A:C2    | 34:RO:22:ILE:HG23  | 2.55                     | 0.42              |
| 7:QG:76:ARG:HH11   | 7:QG:78:ARG:HH12   | 1.67                     | 0.42              |
| 1:XA:600:C:H2'     | 1:XA:601:C:H6      | 1.84                     | 0.42              |
| 29:RF:33:LEU:HD13  | 29:RF:112:MET:HE2  | 2.02                     | 0.42              |
| 1:QA:325:A:H2'     | 1:QA:326:G:O4'     | 2.20                     | 0.42              |
| 30:YG:105:LYS:HD3  | 50:Y4:24:THR:O     | 2.19                     | 0.42              |
| 25:YA:2109:U:H2'   | 25:YA:2110:G:C8    | 2.55                     | 0.42              |
| 1:QA:1182:G:H4'    | 1:QA:1183:A:H5'    | 2.01                     | 0.42              |
| 31:YH:78:GLY:HA2   | 31:YH:83:TYR:CE1   | 2.54                     | 0.42              |
| 46:R0:30:VAL:HG22  | 46:R0:66:VAL:HG22  | 2.02                     | 0.42              |
| 4:XD:190:ASP:OD1   | 4:XD:191:ARG:N     | 2.51                     | 0.42              |
| 25:RA:219:G:C6     | 25:RA:220:G:C6     | 3.08                     | 0.42              |
| 4:XD:50:ARG:HA     | 4:XD:51:PRO:HD3    | 1.77                     | 0.42              |
| 6:QF:96:PRO:HB2    | 6:QF:98:LEU:HD23   | 2.02                     | 0.42              |
| 17:QQ:5:VAL:HG22   | 17:QQ:60:ILE:HG13  | 2.02                     | 0.42              |
| 28:RE:120:TRP:CE3  | 28:RE:155:LYS:HE3  | 2.54                     | 0.42              |
| 45:RZ:81:ARG:HB2   | 45:RZ:81:ARG:HE    | 1.43                     | 0.42              |
| 6:XF:23:LYS:HB3    | 6:XF:23:LYS:HE2    | 1.88                     | 0.42              |
| 8:QH:25:ASP:OD1    | 8:QH:25:ASP:N      | 2.52                     | 0.42              |
| 1:QA:1157:A:N3     | 1:QA:1157:A:H2'    | 2.34                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:RA:1899:G:N3     | 25:RA:1899:G:H2'   | 2.35                     | 0.42              |
| 25:YA:2811:G:H8     | 25:YA:2811:G:OP2   | 2.03                     | 0.42              |
| 45:RZ:103:ARG:HG3   | 45:RZ:104:PHE:H    | 1.85                     | 0.42              |
| 4:QD:50:ARG:HH12    | 5:QE:10:MET:HB3    | 1.84                     | 0.42              |
| 1:QA:1486:G:H2'     | 1:QA:1487:G:O4'    | 2.19                     | 0.42              |
| 25:YA:1991:U:H2'    | 25:YA:1992:G:H5''  | 2.01                     | 0.42              |
| 38:RS:5:THR:OG1     | 38:RS:8:GLU:HG2    | 2.19                     | 0.42              |
| 25:RA:1488:G:H5'    | 25:RA:1489:U:OP2   | 2.20                     | 0.42              |
| 32:RI:142:VAL:HG22  | 32:RI:143:SER:N    | 2.34                     | 0.42              |
| 9:QI:11:LYS:CD      | 9:QI:107:ARG:O     | 2.57                     | 0.42              |
| 25:RA:744:G:H2'     | 25:RA:745:G:O4'    | 2.20                     | 0.42              |
| 2:QB:213:LEU:HD21   | 2:QB:217:ARG:HH12  | 1.84                     | 0.42              |
| 23:QX:10:G:C3'      | 23:QX:11:U:H5''    | 2.50                     | 0.42              |
| 33:YN:56:ASN:HA     | 33:YN:125:GLY:N    | 2.35                     | 0.42              |
| 45:RZ:26:GLY:HA2    | 45:RZ:85:HIS:CD2   | 2.55                     | 0.42              |
| 1:XA:316:G:H2'      | 1:XA:317:G:H8      | 1.84                     | 0.42              |
| 25:RA:128:C:HO2'    | 25:RA:129:C:P      | 2.43                     | 0.42              |
| 25:RA:614(A):U:H5'' | 25:RA:614(B):G:OP1 | 2.20                     | 0.42              |
| 1:QA:953:G:H2'      | 1:QA:954:G:O4'     | 2.20                     | 0.42              |
| 30:RG:27:ASN:HB3    | 30:RG:30:GLU:HG3   | 2.02                     | 0.42              |
| 27:YD:72:LYS:HE3    | 27:YD:99:ASP:OD1   | 2.19                     | 0.42              |
| 25:RA:1628:G:H2'    | 25:RA:1629:U:H6    | 1.84                     | 0.42              |
| 25:RA:2556:C:H2'    | 25:RA:2557:G:O4'   | 2.20                     | 0.42              |
| 22:XW:64:G:H2'      | 22:XW:65:C:O4'     | 2.20                     | 0.42              |
| 20:XT:14:LYS:HA     | 20:XT:17:ARG:NE    | 2.34                     | 0.42              |
| 25:YA:185:U:H2'     | 25:YA:186:G:C8     | 2.54                     | 0.42              |
| 1:XA:1096:C:H2'     | 1:XA:1097:C:H6     | 1.84                     | 0.42              |
| 49:R3:43:ILE:O      | 49:R3:47:VAL:HG23  | 2.19                     | 0.42              |
| 5:QE:48:ALA:HB2     | 5:QE:57:LYS:HD3    | 2.02                     | 0.42              |
| 19:QS:79:THR:O      | 19:QS:81:ARG:N     | 2.53                     | 0.42              |
| 1:XA:644:G:H5'      | 8:XH:92:ARG:HH22   | 1.84                     | 0.42              |
| 25:YA:2410:G:C2     | 25:YA:2411:A:H1'   | 2.54                     | 0.42              |
| 25:RA:590:A:OP1     | 29:RF:95:ARG:NH1   | 2.53                     | 0.42              |
| 1:QA:1422:G:O3'     | 34:RO:49:ARG:NH1   | 2.53                     | 0.42              |
| 49:Y3:35:ARG:HE     | 49:Y3:37:LEU:HD21  | 1.84                     | 0.42              |
| 34:RO:63:VAL:HG12   | 34:RO:106:LEU:HD11 | 2.02                     | 0.42              |
| 25:RA:1184:G:C6     | 25:RA:1185:C:C4    | 3.07                     | 0.42              |
| 33:YN:127:ASP:N     | 33:YN:127:ASP:OD1  | 2.52                     | 0.42              |
| 38:YS:44:LYS:HE3    | 38:YS:44:LYS:HB2   | 1.84                     | 0.42              |
| 1:QA:1069:C:O2'     | 1:QA:1192:C:H1'    | 2.20                     | 0.42              |
| 28:YE:143:ASN:HB2   | 28:YE:147:PRO:HD2  | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1926:U:H2'   | 25:YA:1928:A:OP2   | 2.20                     | 0.42              |
| 25:RA:1576:U:H2'   | 25:RA:1577:C:C6    | 2.55                     | 0.42              |
| 54:R8:32:LEU:HA    | 54:R8:33:ASN:HA    | 1.88                     | 0.42              |
| 31:YH:49:VAL:HG22  | 31:YH:50:VAL:H     | 1.85                     | 0.42              |
| 1:QA:329:A:C6      | 1:QA:332:G:C2      | 3.07                     | 0.42              |
| 1:XA:1304:G:C6     | 1:XA:1305:G:N1     | 2.88                     | 0.42              |
| 25:RA:613:G:N2     | 25:RA:614(C):A:O2' | 2.53                     | 0.42              |
| 25:RA:61:G:H1      | 25:RA:94:C:N4      | 2.11                     | 0.42              |
| 17:XQ:63:ARG:HG2   | 17:XQ:64:PRO:HD2   | 2.02                     | 0.42              |
| 26:RB:56:G:H4'     | 26:RB:57:A:O5'     | 2.19                     | 0.42              |
| 44:RY:60:PHE:HD2   | 44:RY:60:PHE:H     | 1.66                     | 0.42              |
| 9:XI:20:ARG:O      | 9:XI:22:GLY:N      | 2.47                     | 0.42              |
| 3:XC:134:ILE:HG22  | 3:XC:168:ALA:HB3   | 2.01                     | 0.42              |
| 35:YP:134:ALA:O    | 35:YP:138:LEU:HD12 | 2.20                     | 0.42              |
| 3:QC:152:ILE:HB    | 3:QC:199:LYS:HB2   | 2.02                     | 0.42              |
| 25:YA:933:A:H2'    | 25:YA:934:G:O4'    | 2.20                     | 0.42              |
| 25:YA:363(B):G:H2' | 25:YA:363(C):G:C8  | 2.55                     | 0.42              |
| 25:RA:26:G:C6      | 25:RA:27:G:N1      | 2.88                     | 0.42              |
| 25:RA:872:A:OP2    | 36:RQ:5:ARG:NH2    | 2.53                     | 0.42              |
| 25:RA:111:A:H2'    | 25:RA:112:U:O4'    | 2.20                     | 0.42              |
| 11:QK:120:ARG:HA   | 11:QK:121:PRO:HD3  | 1.91                     | 0.42              |
| 16:QP:38:TYR:CZ    | 16:QP:50:LYS:HB3   | 2.55                     | 0.42              |
| 27:RD:43:ARG:HB2   | 27:RD:54:ARG:HB2   | 2.00                     | 0.42              |
| 53:R7:34:ARG:NH1   | 53:R7:41:ARG:O     | 2.53                     | 0.42              |
| 19:QS:35:SER:HB3   | 19:QS:37:ARG:HB2   | 2.02                     | 0.42              |
| 37:YR:5:LYS:HE2    | 37:YR:5:LYS:HB3    | 1.83                     | 0.42              |
| 10:QJ:22:LYS:HB3   | 10:QJ:22:LYS:HE3   | 1.81                     | 0.42              |
| 1:XA:570:G:H1'     | 1:XA:820:U:C4      | 2.55                     | 0.42              |
| 55:Y9:11:CYS:SG    | 55:Y9:27:CYS:SG    | 3.17                     | 0.42              |
| 25:RA:383:U:H2'    | 25:RA:385:C:H5     | 1.85                     | 0.42              |
| 45:RZ:74:VAL:HG22  | 45:RZ:86:VAL:HG13  | 2.01                     | 0.42              |
| 25:YA:706:A:H2'    | 25:YA:707:G:O4'    | 2.19                     | 0.42              |
| 28:RE:78:LEU:HA    | 28:RE:79:ARG:HA    | 1.91                     | 0.42              |
| 25:RA:1348:G:H1    | 25:RA:1598:C:H42   | 1.68                     | 0.42              |
| 39:RT:56:GLY:O     | 39:RT:59:THR:HG22  | 2.20                     | 0.42              |
| 9:QI:31:GLN:HB3    | 9:QI:32:ASP:H      | 1.52                     | 0.42              |
| 43:YX:49:VAL:HG23  | 43:YX:51:VAL:HG23  | 2.02                     | 0.42              |
| 1:QA:485:G:O2'     | 1:QA:486:U:O5'     | 2.33                     | 0.42              |
| 4:QD:21:LEU:O      | 4:QD:23:GLY:N      | 2.53                     | 0.42              |
| 1:XA:1327:C:H2'    | 1:XA:1328:C:H6     | 1.84                     | 0.42              |
| 46:Y0:72:ARG:HB2   | 46:Y0:75:LEU:HB2   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:RA:2023:G:H5'  | 25:RA:2617:C:H4'  | 2.01                     | 0.42              |
| 25:YA:2314:C:H2'  | 25:YA:2315:G:H8   | 1.84                     | 0.42              |
| 26:YB:44:G:H5''   | 26:YB:45:A:OP1    | 2.20                     | 0.42              |
| 1:QA:1300:G:O2'   | 1:QA:1301:U:P     | 2.78                     | 0.42              |
| 30:RG:55:LYS:HD2  | 30:RG:58:GLN:NE2  | 2.34                     | 0.42              |
| 25:RA:1484:G:H1   | 25:RA:1505:C:H42  | 1.67                     | 0.42              |
| 25:RA:519:U:H2'   | 25:RA:520:G:C8    | 2.54                     | 0.42              |
| 25:YA:2823:A:OP1  | 28:YE:113:PHE:HB2 | 2.18                     | 0.42              |
| 12:XL:52:LEU:HA   | 12:XL:52:LEU:HD23 | 1.89                     | 0.42              |
| 1:QA:4:U:O4       | 8:QH:105:ARG:HD3  | 2.20                     | 0.42              |
| 7:XG:18:TYR:CD2   | 7:XG:59:LEU:HD22  | 2.55                     | 0.42              |
| 1:XA:1058:G:H2'   | 1:XA:1059:C:O4'   | 2.19                     | 0.42              |
| 25:RA:580:C:H2'   | 25:RA:581:C:H6    | 1.85                     | 0.42              |
| 25:YA:2183:C:H2'  | 25:YA:2184:G:H8   | 1.85                     | 0.42              |
| 45:RZ:24:LEU:HB2  | 45:RZ:41:LEU:HG   | 2.02                     | 0.42              |
| 22:QW:6:G:H2'     | 22:QW:7:G:C8      | 2.54                     | 0.42              |
| 25:RA:60:G:C5     | 25:RA:63:U:C4     | 3.07                     | 0.42              |
| 28:YE:10:GLY:HA3  | 39:YT:8:LYS:HD2   | 2.02                     | 0.42              |
| 36:YQ:88:GLY:O    | 36:YQ:90:VAL:N    | 2.52                     | 0.42              |
| 55:Y9:4:ARG:O     | 55:Y9:36:GLN:HA   | 2.20                     | 0.42              |
| 15:XO:21:ASP:OD1  | 15:XO:24:SER:HB2  | 2.20                     | 0.42              |
| 42:RW:31:GLU:O    | 42:RW:35:ILE:HG13 | 2.19                     | 0.42              |
| 25:YA:947:G:N3    | 25:YA:984:A:H2    | 2.18                     | 0.42              |
| 25:RA:2259:G:C2   | 25:RA:2282:G:C6   | 3.08                     | 0.42              |
| 1:QA:1154:G:H2'   | 1:QA:1155:G:H8    | 1.84                     | 0.42              |
| 39:RT:80:SER:HB3  | 39:RT:83:ILE:HG13 | 2.00                     | 0.42              |
| 29:YF:61:GLY:C    | 29:YF:77:ASP:HB3  | 2.40                     | 0.42              |
| 25:YA:2070:G:C2   | 25:YA:2071:A:C4   | 3.08                     | 0.42              |
| 5:QE:71:LEU:HD11  | 5:QE:114:GLY:HA3  | 2.01                     | 0.42              |
| 52:R6:30:THR:HA   | 52:R6:31:PRO:C    | 2.40                     | 0.42              |
| 1:QA:1284:C:H3'   | 1:QA:1285:A:H8    | 1.83                     | 0.42              |
| 25:RA:192:C:O2'   | 25:RA:802:A:N3    | 2.45                     | 0.42              |
| 20:QT:38:LYS:HE2  | 20:QT:38:LYS:HB3  | 1.73                     | 0.42              |
| 2:XB:108:ILE:HD13 | 2:XB:108:ILE:HA   | 1.80                     | 0.42              |
| 1:XA:198:G:H2'    | 1:XA:199:G:H8     | 1.84                     | 0.42              |
| 7:QG:116:ALA:O    | 7:QG:120:ILE:HG12 | 2.19                     | 0.42              |
| 25:RA:1002:G:H2'  | 25:RA:1003:G:O4'  | 2.20                     | 0.42              |
| 30:YG:121:ASN:HA  | 30:YG:122:PRO:HD2 | 1.92                     | 0.42              |
| 31:RH:7:LEU:HD13  | 31:RH:69:ARG:CB   | 2.45                     | 0.42              |
| 44:YY:101:LYS:HB3 | 44:YY:101:LYS:HE2 | 1.81                     | 0.42              |
| 44:YY:76:CYS:HB3  | 44:YY:96:ILE:HD11 | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:RZ:126:VAL:HG12 | 45:RZ:163:LEU:HD13 | 2.01                     | 0.42              |
| 25:YA:996:A:O2'    | 40:YU:92:ARG:NE    | 2.52                     | 0.42              |
| 35:YP:124:LYS:HA   | 35:YP:143:GLY:O    | 2.19                     | 0.42              |
| 4:QD:200:GLU:O     | 4:QD:204:ILE:HG12  | 2.20                     | 0.42              |
| 1:XA:315:A:O2'     | 1:XA:316:G:P       | 2.78                     | 0.42              |
| 1:XA:410:G:H4'     | 1:XA:411:A:OP1     | 2.19                     | 0.42              |
| 25:RA:2476:A:H62   | 25:RA:2477:C:N4    | 2.18                     | 0.42              |
| 26:RB:56:G:H4'     | 26:RB:57:A:H8      | 1.84                     | 0.42              |
| 1:QA:971:G:H21     | 1:QA:1233:G:H1'    | 1.84                     | 0.42              |
| 44:YY:89:PHE:O     | 44:YY:90:LEU:HD22  | 2.20                     | 0.42              |
| 44:YY:88:LYS:C     | 44:YY:90:LEU:H     | 2.21                     | 0.42              |
| 22:XW:36:U:H2'     | 22:XW:37:A:C8      | 2.55                     | 0.42              |
| 2:XB:34:ALA:O      | 2:XB:41:ILE:HB     | 2.20                     | 0.42              |
| 1:XA:1273:G:H3'    | 1:XA:1274:G:C8     | 2.53                     | 0.42              |
| 25:YA:270(Q):C:O3' | 32:YI:42:SER:OG    | 2.34                     | 0.42              |
| 1:XA:779:C:O2'     | 11:XK:120:ARG:HD3  | 2.19                     | 0.42              |
| 22:XW:7:G:H5''     | 22:XW:8:U:OP2      | 2.20                     | 0.42              |
| 31:YH:22:GLY:C     | 31:YH:37:VAL:HB    | 2.39                     | 0.42              |
| 5:QE:112:LEU:HA    | 5:QE:112:LEU:HD23  | 1.86                     | 0.42              |
| 25:RA:861:A:H2'    | 25:RA:862:G:O5'    | 2.19                     | 0.42              |
| 4:XD:187:ARG:NH2   | 4:XD:193:ASP:OD1   | 2.53                     | 0.42              |
| 22:QW:1:C:N4       | 22:QW:2:G:O6       | 2.53                     | 0.42              |
| 25:RA:634:C:H2'    | 25:RA:635:C:C6     | 2.55                     | 0.42              |
| 25:RA:2283:C:OP2   | 52:R6:6:ARG:HB2    | 2.20                     | 0.42              |
| 1:XA:1143:G:H2'    | 1:XA:1144:G:H8     | 1.84                     | 0.42              |
| 25:RA:1853:A:N1    | 25:RA:2087:G:H1'   | 2.35                     | 0.42              |
| 1:QA:1353:G:H2'    | 1:QA:1354:C:H6     | 1.84                     | 0.42              |
| 44:YY:29:GLU:HB3   | 44:YY:38:ILE:HG23  | 2.02                     | 0.42              |
| 25:RA:13:A:N1      | 25:RA:525:U:H2'    | 2.35                     | 0.42              |
| 24:QY:67:THR:HG23  | 24:QY:73:ARG:NH1   | 2.34                     | 0.42              |
| 39:YT:88:ILE:O     | 39:YT:88:ILE:HG13  | 2.20                     | 0.42              |
| 28:RE:76:ARG:HD2   | 28:RE:76:ARG:N     | 2.35                     | 0.42              |
| 30:YG:111:LEU:HB2  | 30:YG:112:PRO:HD3  | 2.02                     | 0.42              |
| 1:QA:1057:G:H4'    | 3:QC:196:LEU:HA    | 2.02                     | 0.42              |
| 31:YH:51:ARG:HG3   | 31:YH:51:ARG:H     | 1.41                     | 0.41              |
| 35:RP:144:GLU:OE1  | 35:RP:144:GLU:N    | 2.52                     | 0.41              |
| 35:YP:70:GLN:HB3   | 35:YP:71:VAL:H     | 1.72                     | 0.41              |
| 25:YA:1301:A:C8    | 25:YA:1303:G:C8    | 3.08                     | 0.41              |
| 12:XL:33:ARG:HD3   | 12:XL:62:SER:OG    | 2.20                     | 0.41              |
| 25:YA:1007:C:H5''  | 33:YN:35:ARG:NH1   | 2.34                     | 0.41              |
| 29:YF:116:ASP:OD1  | 29:YF:119:ARG:NH2  | 2.53                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:XD:104:VAL:O    | 4:XD:108:LEU:HB2  | 2.21                     | 0.41              |
| 25:RA:957:A:N1    | 25:RA:2458:G:H4'  | 2.35                     | 0.41              |
| 42:RW:17:VAL:O    | 42:RW:20:VAL:HG22 | 2.20                     | 0.41              |
| 30:RG:53:LEU:HD13 | 30:RG:87:PRO:HB2  | 2.01                     | 0.41              |
| 22:XW:53:G:H1     | 22:XW:61:C:N4     | 2.18                     | 0.41              |
| 1:XA:1260:C:H6    | 1:XA:1260:C:H5''  | 1.85                     | 0.41              |
| 27:YD:102:LYS:C   | 27:YD:103:ARG:HG2 | 2.41                     | 0.41              |
| 1:XA:33:A:H2'     | 1:XA:34:C:H6      | 1.84                     | 0.41              |
| 41:YV:79:VAL:O    | 41:YV:80:GLN:HB2  | 2.19                     | 0.41              |
| 38:YS:5:THR:OG1   | 38:YS:8:GLU:HG2   | 2.20                     | 0.41              |
| 3:XC:112:SER:O    | 3:XC:116:VAL:HG23 | 2.20                     | 0.41              |
| 25:YA:959:A:N6    | 36:YQ:82:ARG:HH12 | 2.18                     | 0.41              |
| 29:YF:46:ARG:HG2  | 29:YF:46:ARG:HH11 | 1.83                     | 0.41              |
| 55:R9:2:LYS:HD2   | 55:R9:33:LYS:O    | 2.19                     | 0.41              |
| 1:XA:585:G:H4'    | 12:XL:8:ASN:OD1   | 2.20                     | 0.41              |
| 43:RX:60:ARG:O    | 43:RX:75:ASP:HB3  | 2.20                     | 0.41              |
| 15:XO:12:ILE:HG12 | 15:XO:31:LEU:HD11 | 2.01                     | 0.41              |
| 25:YA:1952:A:C2   | 34:YO:22:ILE:HG23 | 2.55                     | 0.41              |
| 25:YA:687:C:H2'   | 25:YA:688:U:O4'   | 2.20                     | 0.41              |
| 15:XO:43:LEU:HD11 | 15:XO:53:HIS:HA   | 2.01                     | 0.41              |
| 32:RI:10:GLU:OE1  | 32:RI:11:ASN:N    | 2.53                     | 0.41              |
| 1:QA:21:G:H2'     | 1:QA:22:G:C8      | 2.55                     | 0.41              |
| 7:QG:65:ALA:O     | 7:QG:69:VAL:HG23  | 2.20                     | 0.41              |
| 28:RE:55:ASN:ND2  | 28:RE:75:VAL:HG22 | 2.36                     | 0.41              |
| 1:XA:536:C:H2'    | 1:XA:537:G:C8     | 2.55                     | 0.41              |
| 38:RS:93:LYS:HB2  | 38:RS:93:LYS:HE3  | 1.90                     | 0.41              |
| 8:QH:6:ILE:H      | 8:QH:6:ILE:HD12   | 1.85                     | 0.41              |
| 1:XA:1372:U:H2'   | 1:XA:1373:G:O4'   | 2.19                     | 0.41              |
| 35:RP:79:ARG:NE   | 35:RP:109:GLY:HA3 | 2.35                     | 0.41              |
| 48:R2:13:ALA:HB1  | 48:R2:21:LEU:HD21 | 2.02                     | 0.41              |
| 1:XA:818:G:O3'    | 1:XA:819:A:H4'    | 2.20                     | 0.41              |
| 25:YA:43:G:H2'    | 25:YA:44:A:O4'    | 2.20                     | 0.41              |
| 28:RE:79:ARG:O    | 28:RE:80:GLU:CG   | 2.68                     | 0.41              |
| 19:QS:36:ARG:HH22 | 19:QS:69:HIS:HA   | 1.85                     | 0.41              |
| 25:YA:2103:C:N4   | 25:YA:2104:G:O6   | 2.52                     | 0.41              |
| 22:QW:50:U:H2'    | 22:QW:51:C:C6     | 2.55                     | 0.41              |
| 21:XU:9:ARG:NH2   | 21:XU:10:ARG:HE   | 2.18                     | 0.41              |
| 38:YS:62:LYS:HB3  | 38:YS:97:ARG:CD   | 2.49                     | 0.41              |
| 4:XD:20:TYR:CE2   | 4:XD:27:TYR:HA    | 2.55                     | 0.41              |
| 27:RD:92:ILE:HD12 | 27:RD:104:TYR:CE2 | 2.55                     | 0.41              |
| 1:QA:735:C:H2'    | 1:QA:736:C:C6     | 2.54                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:YA:1270:C:C5'   | 25:YA:1271:G:H5'   | 2.49                     | 0.41              |
| 25:RA:990:A:H5'    | 25:RA:990:A:H8     | 1.85                     | 0.41              |
| 39:RT:6:LEU:HA     | 39:RT:6:LEU:HD12   | 1.95                     | 0.41              |
| 2:QB:97:TRP:CE2    | 2:QB:101:MET:HG3   | 2.56                     | 0.41              |
| 25:YA:2145:C:H5''  | 25:YA:2146:C:C5    | 2.55                     | 0.41              |
| 25:YA:882:G:H1     | 25:YA:894:C:H42    | 1.68                     | 0.41              |
| 48:Y2:46:GLN:HB2   | 48:Y2:49:LYS:NZ    | 2.34                     | 0.41              |
| 35:YP:144:GLU:HA   | 35:YP:145:PRO:HD3  | 1.80                     | 0.41              |
| 12:QL:57:LYS:HE3   | 12:QL:65:GLU:HG2   | 2.01                     | 0.41              |
| 30:RG:111:LEU:HD13 | 30:RG:120:LEU:HD21 | 2.01                     | 0.41              |
| 2:XB:17:PHE:HD2    | 2:XB:41:ILE:HG23   | 1.85                     | 0.41              |
| 11:XK:29:ILE:HD13  | 11:XK:29:ILE:HG21  | 1.80                     | 0.41              |
| 4:XD:107:ARG:HH21  | 4:XD:194:LEU:HD12  | 1.85                     | 0.41              |
| 1:XA:1055:A:O2'    | 3:XC:161:GLU:OE2   | 2.30                     | 0.41              |
| 20:QT:26:ASN:O     | 20:QT:30:LYS:HB2   | 2.19                     | 0.41              |
| 1:XA:1517:G:H1'    | 25:YA:1919:A:O3'   | 2.19                     | 0.41              |
| 25:YA:1278:A:H5''  | 37:YR:36:THR:HG22  | 2.02                     | 0.41              |
| 25:YA:708:C:H5'    | 25:YA:709:U:OP2    | 2.20                     | 0.41              |
| 25:YA:154:G:C6     | 25:YA:155:C:N4     | 2.88                     | 0.41              |
| 35:RP:6:LEU:HB3    | 35:RP:7:ARG:H      | 1.61                     | 0.41              |
| 36:YQ:81:VAL:HG12  | 36:YQ:82:ARG:HG2   | 2.02                     | 0.41              |
| 26:YB:29:A:H2'     | 26:YB:30:C:C6      | 2.55                     | 0.41              |
| 38:RS:10:ARG:O     | 38:RS:14:VAL:HG12  | 2.20                     | 0.41              |
| 1:XA:246:A:N6      | 1:XA:281:G:H1'     | 2.35                     | 0.41              |
| 13:XM:50:GLU:O     | 13:XM:54:VAL:HG23  | 2.20                     | 0.41              |
| 36:RQ:137:TYR:CE1  | 45:RZ:83:PRO:HG3   | 2.55                     | 0.41              |
| 31:YH:159:GLU:HB3  | 31:YH:160:LYS:H    | 1.55                     | 0.41              |
| 28:RE:103:ASP:OD1  | 28:RE:201:THR:HG23 | 2.19                     | 0.41              |
| 47:R1:91:LYS:C     | 47:R1:93:GLU:H     | 2.23                     | 0.41              |
| 8:QH:50:ARG:HA     | 8:QH:59:LEU:HD23   | 2.02                     | 0.41              |
| 27:RD:25:THR:HG21  | 27:RD:82:ILE:H     | 1.84                     | 0.41              |
| 25:YA:1062:G:H2'   | 25:YA:1063:G:H8    | 1.85                     | 0.41              |
| 50:R4:13:ARG:HD3   | 50:R4:13:ARG:HA    | 1.86                     | 0.41              |
| 28:RE:57:LYS:HA    | 28:RE:57:LYS:HD2   | 1.84                     | 0.41              |
| 1:QA:812:C:H2'     | 1:QA:812:C:H6      | 1.62                     | 0.41              |
| 28:YE:81:ILE:HG21  | 28:YE:84:PHE:CD1   | 2.55                     | 0.41              |
| 25:YA:1726:G:C6    | 25:YA:1727:U:C4    | 3.08                     | 0.41              |
| 44:YY:43:ASN:HB3   | 44:YY:64:GLU:HA    | 2.03                     | 0.41              |
| 32:YI:1:MET:HB3    | 32:YI:21:VAL:O     | 2.21                     | 0.41              |
| 1:QA:685:G:C2      | 1:QA:686:U:C4      | 3.08                     | 0.41              |
| 45:RZ:59:LEU:HD12  | 45:RZ:60:GLU:C     | 2.41                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:YE:60:ASN:O     | 28:YE:62:PRO:CD    | 2.68                     | 0.41              |
| 41:RV:85:LYS:HG3   | 41:RV:87:HIS:HA    | 2.02                     | 0.41              |
| 13:QM:86:CYS:HB2   | 19:QS:73:GLU:HB3   | 2.02                     | 0.41              |
| 27:YD:34:VAL:C     | 27:YD:35:LYS:HG3   | 2.40                     | 0.41              |
| 35:YP:12:ALA:C     | 35:YP:14:LYS:H     | 2.23                     | 0.41              |
| 1:QA:590:C:H2'     | 1:QA:591:U:C6      | 2.54                     | 0.41              |
| 19:XS:35:SER:HB3   | 19:XS:37:ARG:HB2   | 2.02                     | 0.41              |
| 1:XA:826:C:H2'     | 1:XA:827:U:C6      | 2.55                     | 0.41              |
| 31:RH:170:ARG:HB3  | 31:RH:171:LEU:H    | 1.57                     | 0.41              |
| 13:QM:118:ALA:CB   | 22:QV:29:G:H5'     | 2.49                     | 0.41              |
| 25:RA:582:G:H2'    | 25:RA:583:G:H8     | 1.84                     | 0.41              |
| 25:RA:1408:C:C2    | 25:RA:1595:G:N2    | 2.88                     | 0.41              |
| 1:QA:8:A:N6        | 4:QD:209:ARG:HB2   | 2.35                     | 0.41              |
| 27:RD:133:LEU:HD12 | 27:RD:189:CYS:HB2  | 2.01                     | 0.41              |
| 31:RH:136:ILE:O    | 31:RH:137:ASP:HB2  | 2.21                     | 0.41              |
| 25:RA:956:G:H2'    | 25:RA:957:A:H2'    | 2.02                     | 0.41              |
| 1:QA:1007:C:H42    | 1:QA:1022:G:H1     | 1.69                     | 0.41              |
| 38:YS:93:LYS:HE3   | 38:YS:93:LYS:HB2   | 1.75                     | 0.41              |
| 9:QI:2:GLU:O       | 9:QI:20:ARG:NH1    | 2.53                     | 0.41              |
| 25:RA:638:G:C6     | 25:RA:639:U:C4     | 3.08                     | 0.41              |
| 1:QA:411:A:H2'     | 1:QA:412:A:H4'     | 2.01                     | 0.41              |
| 1:XA:187:C:O2'     | 20:XT:89:ARG:NE    | 2.51                     | 0.41              |
| 25:RA:2773:C:H2'   | 25:RA:2774:C:H6    | 1.85                     | 0.41              |
| 32:RI:73:GLU:OE1   | 32:RI:137:PRO:HD2  | 2.21                     | 0.41              |
| 25:YA:1858:G:H1'   | 25:YA:1884:A:N6    | 2.34                     | 0.41              |
| 1:QA:186:C:H1'     | 20:QT:81:LYS:HE3   | 2.01                     | 0.41              |
| 25:YA:479:A:HO2'   | 25:YA:481:G:H8     | 1.66                     | 0.41              |
| 45:YZ:53:ILE:HA    | 45:YZ:71:VAL:HG13  | 2.02                     | 0.41              |
| 36:YQ:134:ARG:HH21 | 45:YZ:122:ARG:NH1  | 2.18                     | 0.41              |
| 7:QG:76:ARG:O      | 7:QG:87:VAL:N      | 2.52                     | 0.41              |
| 47:R1:97:LEU:HD13  | 47:R1:97:LEU:HA    | 1.91                     | 0.41              |
| 1:XA:201:C:O2'     | 1:XA:202:U:OP1     | 2.32                     | 0.41              |
| 26:RB:8:U:O3'      | 38:RS:25:ARG:NH2   | 2.53                     | 0.41              |
| 1:XA:765:G:N1      | 1:XA:812:C:H1'     | 2.36                     | 0.41              |
| 27:YD:165:ILE:H    | 27:YD:165:ILE:HG12 | 1.61                     | 0.41              |
| 25:RA:724:U:H2'    | 25:RA:725:G:O4'    | 2.20                     | 0.41              |
| 5:QE:51:VAL:O      | 5:QE:55:VAL:HG23   | 2.19                     | 0.41              |
| 25:RA:1362:C:O2'   | 25:RA:1363:C:H5'   | 2.20                     | 0.41              |
| 5:QE:70:PRO:O      | 5:QE:72:GLN:NE2    | 2.53                     | 0.41              |
| 4:XD:64:LEU:HD23   | 4:XD:75:PHE:HZ     | 1.85                     | 0.41              |
| 24:QY:49:GLN:O     | 24:QY:52:LYS:HE3   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:YA:1885:A:H2'  | 25:YA:1886:C:O4'  | 2.21                     | 0.41              |
| 25:RA:1358:G:O2'  | 25:RA:1359:A:H5'' | 2.20                     | 0.41              |
| 25:RA:1385:G:H4'  | 25:RA:1385:G:OP1  | 2.21                     | 0.41              |
| 1:XA:56:U:H2'     | 1:XA:57:G:C8      | 2.54                     | 0.41              |
| 1:XA:109:A:C6     | 1:XA:326:G:C6     | 3.08                     | 0.41              |
| 25:YA:191:A:H2'   | 25:YA:192:C:C6    | 2.55                     | 0.41              |
| 12:QL:45:PRO:HD3  | 12:QL:51:ALA:O    | 2.20                     | 0.41              |
| 1:QA:688:G:H2'    | 1:QA:689:C:H6     | 1.84                     | 0.41              |
| 25:YA:631:A:H2'   | 25:YA:632:A:O4'   | 2.20                     | 0.41              |
| 44:YY:95:LYS:NZ   | 44:YY:95:LYS:HB2  | 2.35                     | 0.41              |
| 9:QI:118:LYS:O    | 9:QI:120:ARG:N    | 2.53                     | 0.41              |
| 19:QS:36:ARG:HD2  | 19:QS:71:LEU:N    | 2.21                     | 0.41              |
| 22:XV:53:G:N2     | 22:XV:61:C:O2     | 2.53                     | 0.41              |
| 25:RA:2712:U:H5   | 25:RA:2715:C:OP1  | 2.04                     | 0.41              |
| 25:YA:6:A:C8      | 25:YA:6:A:O5'     | 2.74                     | 0.41              |
| 40:RU:98:LEU:C    | 40:RU:100:VAL:N   | 2.74                     | 0.41              |
| 1:QA:316:G:OP2    | 1:QA:351:G:O2'    | 2.37                     | 0.41              |
| 25:RA:1754:C:OP2  | 39:RT:113:LYS:HE3 | 2.20                     | 0.41              |
| 25:RA:2198:A:O2'  | 25:RA:2199:A:C8   | 2.72                     | 0.41              |
| 34:YO:68:GLU:HB3  | 34:YO:78:ARG:HB2  | 2.02                     | 0.41              |
| 50:Y4:58:ARG:O    | 50:Y4:62:ARG:HG2  | 2.20                     | 0.41              |
| 1:XA:1313:U:OP2   | 19:XS:6:LYS:HB3   | 2.19                     | 0.41              |
| 48:R2:15:LYS:HA   | 48:R2:15:LYS:HD3  | 1.93                     | 0.41              |
| 2:QB:221:LEU:HA   | 2:QB:224:GLN:HB2  | 2.00                     | 0.41              |
| 51:R5:25:LEU:HA   | 51:R5:25:LEU:HD23 | 1.88                     | 0.41              |
| 25:RA:2173:A:C5   | 25:RA:2174:C:H1'  | 2.54                     | 0.41              |
| 25:YA:2420:C:N4   | 54:Y8:31:HIS:HA   | 2.35                     | 0.41              |
| 7:XG:76:ARG:HB3   | 7:XG:78:ARG:HH11  | 1.84                     | 0.41              |
| 2:XB:126:GLU:O    | 2:XB:130:ARG:NH1  | 2.53                     | 0.41              |
| 10:QJ:27:ALA:HB2  | 10:QJ:85:LEU:HD11 | 2.03                     | 0.41              |
| 38:YS:11:LYS:HD3  | 38:YS:91:PRO:HD3  | 2.02                     | 0.41              |
| 2:XB:93:VAL:HG11  | 2:XB:97:TRP:HD1   | 1.85                     | 0.41              |
| 38:RS:14:VAL:HG21 | 38:RS:89:ARG:HB3  | 2.02                     | 0.41              |
| 5:QE:69:VAL:HA    | 5:QE:70:PRO:HD2   | 1.92                     | 0.41              |
| 1:XA:1317:C:OP1   | 14:XN:17:LYS:HG2  | 2.20                     | 0.41              |
| 25:RA:973:A:H5'   | 25:RA:1188:U:H1'  | 2.01                     | 0.41              |
| 25:YA:2074:U:H2'  | 25:YA:2075:U:C6   | 2.54                     | 0.41              |
| 25:RA:971:C:O2'   | 25:RA:983:A:N3    | 2.44                     | 0.41              |
| 25:RA:1465:G:H5'  | 25:RA:1528:A:O2'  | 2.21                     | 0.41              |
| 2:XB:22:LYS:HB3   | 2:XB:23:ARG:H     | 1.70                     | 0.41              |
| 25:YA:627:A:OP2   | 25:YA:627:A:H8    | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:XR:51:LEU:HD23  | 18:XR:51:LEU:HA    | 1.92                     | 0.41              |
| 2:XB:29:ALA:HB1    | 2:XB:30:ARG:HH21   | 1.85                     | 0.41              |
| 31:YH:85:LYS:HA    | 31:YH:85:LYS:HD2   | 1.62                     | 0.41              |
| 7:QG:104:LEU:HD13  | 7:QG:104:LEU:HA    | 1.91                     | 0.41              |
| 28:RE:203:LYS:HE3  | 28:RE:203:LYS:HB2  | 1.80                     | 0.41              |
| 22:QV:23:C:H2'     | 22:QV:24:U:C6      | 2.55                     | 0.41              |
| 41:RV:1:MET:N      | 41:RV:16:PRO:HD3   | 2.36                     | 0.41              |
| 40:RU:28:ARG:NH1   | 40:RU:38:THR:OG1   | 2.45                     | 0.41              |
| 25:RA:2061:G:H5''  | 25:RA:2503:A:C2    | 2.55                     | 0.41              |
| 25:RA:2748:A:H2    | 25:RA:2754:U:H3    | 1.65                     | 0.41              |
| 28:RE:79:ARG:HH11  | 28:RE:164:ARG:HH12 | 1.68                     | 0.41              |
| 4:XD:9:CYS:SG      | 4:XD:32:ALA:HB2    | 2.60                     | 0.41              |
| 35:YP:10:PRO:HB2   | 35:YP:11:GLY:H     | 1.66                     | 0.41              |
| 12:XL:93:LEU:HA    | 12:XL:94:PRO:HD2   | 1.91                     | 0.41              |
| 25:RA:996:A:H4'    | 40:RU:92:ARG:NE    | 2.36                     | 0.41              |
| 29:YF:7:TYR:HA     | 29:YF:125:LEU:O    | 2.21                     | 0.41              |
| 29:RF:53:THR:HG22  | 29:RF:56:GLU:HG3   | 2.01                     | 0.41              |
| 28:YE:38:THR:O     | 28:YE:42:ASP:N     | 2.53                     | 0.41              |
| 30:YG:114:ILE:HG12 | 30:YG:140:ILE:HG21 | 2.02                     | 0.41              |
| 27:RD:108:PRO:HB3  | 27:RD:143:HIS:NE2  | 2.35                     | 0.41              |
| 25:RA:141:A:H8     | 25:RA:1408:C:O2'   | 2.01                     | 0.41              |
| 48:Y2:21:LEU:HD11  | 48:Y2:63:VAL:HG12  | 2.03                     | 0.41              |
| 2:XB:217:ARG:HA    | 2:XB:220:ASP:HB2   | 2.02                     | 0.41              |
| 1:XA:652:U:H1'     | 1:XA:653:A:H2      | 1.84                     | 0.41              |
| 30:RG:76:SER:OG    | 30:RG:83:ARG:HA    | 2.19                     | 0.41              |
| 1:XA:250:A:H5'     | 1:XA:252:U:O4'     | 2.20                     | 0.41              |
| 25:RA:1794:U:H2'   | 25:RA:1795:C:C6    | 2.56                     | 0.41              |
| 25:YA:363(F):A:H8  | 25:YA:363(F):A:OP2 | 2.03                     | 0.41              |
| 1:QA:793:U:OP2     | 1:QA:794:A:H8      | 2.03                     | 0.41              |
| 41:YV:38:LEU:HD12  | 41:YV:55:ALA:HB1   | 2.03                     | 0.41              |
| 25:RA:485:C:H2'    | 25:RA:486:C:C6     | 2.56                     | 0.41              |
| 28:YE:114:ALA:HB3  | 28:YE:160:TYR:HB3  | 2.02                     | 0.41              |
| 1:XA:1041:A:H2'    | 1:XA:1042:G:O4'    | 2.20                     | 0.41              |
| 16:QP:34:GLU:OE2   | 16:QP:55:ARG:HD3   | 2.21                     | 0.41              |
| 25:YA:950:G:C6     | 25:YA:951:C:C4     | 3.09                     | 0.41              |
| 1:XA:1504:G:OP1    | 1:XA:1507:A:H4'    | 2.20                     | 0.41              |
| 25:YA:2341:G:N2    | 25:YA:2374:C:O3'   | 2.54                     | 0.41              |
| 29:YF:32:LEU:O     | 29:YF:36:VAL:HG23  | 2.21                     | 0.41              |
| 25:RA:2186:G:H2'   | 25:RA:2187:G:H8    | 1.85                     | 0.41              |
| 39:YT:33:LYS:O     | 39:YT:82:LEU:HD23  | 2.20                     | 0.41              |
| 27:YD:201:HIS:O    | 27:YD:204:ILE:HG12 | 2.21                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:374:A:C6      | 1:QA:375:U:C4     | 3.08                     | 0.41              |
| 17:XQ:19:VAL:HG23  | 17:XQ:44:ALA:HB3  | 2.03                     | 0.41              |
| 25:RA:1354:A:H2'   | 25:RA:1355:G:O4'  | 2.21                     | 0.41              |
| 9:QI:56:LEU:H      | 9:QI:56:LEU:HD23  | 1.85                     | 0.41              |
| 13:XM:108:ARG:HA   | 13:XM:108:ARG:HD2 | 1.89                     | 0.41              |
| 25:YA:897:C:P      | 25:YA:897:C:H6    | 2.43                     | 0.41              |
| 27:YD:145:VAL:HG12 | 27:YD:146:GLU:O   | 2.20                     | 0.41              |
| 25:YA:1284:A:H2'   | 25:YA:1285:G:O4'  | 2.21                     | 0.41              |
| 25:YA:256:A:H2'    | 25:YA:257:A:H8    | 1.85                     | 0.41              |
| 41:RV:41:GLY:H     | 41:RV:46:VAL:HG13 | 1.85                     | 0.41              |
| 41:RV:50:PRO:C     | 41:RV:51:VAL:HG23 | 2.41                     | 0.41              |
| 32:YI:77:LEU:HB2   | 32:YI:141:LYS:HB2 | 2.03                     | 0.41              |
| 25:RA:2635:C:OP1   | 28:RE:78:LEU:CD1  | 2.68                     | 0.41              |
| 1:QA:1347:G:C2'    | 1:QA:1348:U:OP2   | 2.68                     | 0.41              |
| 25:RA:1696:G:H2'   | 25:RA:1697:G:C5'  | 2.50                     | 0.41              |
| 25:YA:2103:C:H2'   | 25:YA:2104:G:C8   | 2.55                     | 0.41              |
| 22:QW:19:G:C2      | 25:RA:2112:G:N2   | 2.88                     | 0.41              |
| 52:R6:14:THR:OG1   | 52:R6:19:ARG:HA   | 2.19                     | 0.41              |
| 1:QA:345:C:H1'     | 1:QA:346:G:N1     | 2.35                     | 0.41              |
| 25:RA:2091:U:H3'   | 25:RA:2092:U:H5'' | 2.03                     | 0.41              |
| 50:Y4:40:HIS:H     | 50:Y4:41:PRO:CD   | 2.31                     | 0.41              |
| 25:RA:997:G:OP1    | 40:RU:93:LYS:HD2  | 2.21                     | 0.41              |
| 9:QI:83:ARG:HH21   | 9:QI:102:LEU:HD21 | 1.86                     | 0.41              |
| 1:XA:1313:U:P      | 19:XS:6:LYS:HD3   | 2.60                     | 0.41              |
| 52:Y6:14:THR:HG22  | 52:Y6:50:ARG:O    | 2.20                     | 0.41              |
| 18:QR:22:VAL:CG1   | 18:QR:56:THR:HA   | 2.48                     | 0.41              |
| 1:QA:554:C:OP2     | 12:QL:23:LYS:NZ   | 2.46                     | 0.41              |
| 2:XB:55:PHE:CE1    | 2:XB:218:ALA:HA   | 2.56                     | 0.41              |
| 45:RZ:15:PRO:O     | 45:RZ:19:ARG:HB2  | 2.21                     | 0.41              |
| 31:RH:103:LEU:HD13 | 31:RH:123:PHE:HB3 | 2.02                     | 0.41              |
| 25:RA:522:G:H2'    | 25:RA:523:C:C6    | 2.56                     | 0.41              |
| 39:YT:27:THR:CG2   | 39:YT:90:GLN:HB3  | 2.50                     | 0.41              |
| 13:QM:23:TYR:CD2   | 13:QM:70:LEU:HD11 | 2.56                     | 0.41              |
| 44:YY:88:LYS:HA    | 44:YY:88:LYS:HD3  | 1.93                     | 0.41              |
| 25:YA:1380:G:N2    | 25:YA:1570:A:N1   | 2.64                     | 0.41              |
| 10:XJ:20:ALA:O     | 10:XJ:24:VAL:HG23 | 2.21                     | 0.41              |
| 10:XJ:54:PHE:CG    | 10:XJ:55:LYS:HG3  | 2.55                     | 0.41              |
| 25:RA:1952:A:C5    | 34:RO:22:ILE:HD12 | 2.56                     | 0.41              |
| 25:YA:1421:G:C2    | 25:YA:1422:G:C8   | 3.09                     | 0.41              |
| 25:YA:1188:U:O2'   | 25:YA:1189:A:H5'  | 2.21                     | 0.41              |
| 1:XA:1402:C:H2'    | 1:XA:1403:C:O4'   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:QA:41:G:H2'     | 1:QA:42:G:H8       | 1.84                     | 0.41              |
| 34:RO:1:MET:HB2   | 34:RO:32:TYR:HB3   | 2.02                     | 0.41              |
| 38:RS:14:VAL:HG11 | 38:RS:90:GLY:O     | 2.20                     | 0.41              |
| 25:RA:1035:U:H2'  | 25:RA:1036:G:O5'   | 2.21                     | 0.41              |
| 15:QO:29:VAL:HG11 | 15:QO:67:LEU:HD21  | 2.02                     | 0.41              |
| 3:QC:47:LEU:HD21  | 3:QC:68:VAL:HG11   | 2.02                     | 0.41              |
| 38:RS:78:LEU:HD11 | 38:RS:107:GLU:HG3  | 2.02                     | 0.41              |
| 25:YA:1587:A:H2'  | 25:YA:1588:C:C6    | 2.55                     | 0.41              |
| 25:YA:1586:A:C3'  | 25:YA:1587:A:H5'   | 2.51                     | 0.41              |
| 24:QY:31:ASN:O    | 24:QY:35:GLN:HG2   | 2.20                     | 0.41              |
| 8:XH:13:ILE:O     | 8:XH:17:THR:HG23   | 2.21                     | 0.41              |
| 25:RA:1321:A:H2'  | 25:RA:1322:A:O4'   | 2.21                     | 0.41              |
| 6:QF:12:PRO:HD3   | 6:QF:58:GLY:HA2    | 2.03                     | 0.41              |
| 13:XM:66:LEU:HA   | 13:XM:70:LEU:HD12  | 2.02                     | 0.41              |
| 1:QA:811:C:H4'    | 1:QA:900:A:N6      | 2.36                     | 0.41              |
| 25:RA:1259:G:H2'  | 25:RA:1260:G:C8    | 2.55                     | 0.41              |
| 39:RT:50:ILE:HD12 | 39:RT:50:ILE:HA    | 1.88                     | 0.41              |
| 35:YP:98:GLU:H    | 35:YP:98:GLU:HG3   | 1.34                     | 0.41              |
| 4:QD:61:LYS:HB3   | 4:QD:61:LYS:HE3    | 1.89                     | 0.41              |
| 24:XY:34:LEU:HD23 | 24:XY:34:LEU:HA    | 1.90                     | 0.41              |
| 38:RS:15:ARG:HA   | 38:RS:15:ARG:HD3   | 1.93                     | 0.41              |
| 3:QC:12:LEU:HA    | 3:QC:12:LEU:HD23   | 1.90                     | 0.41              |
| 1:XA:1053:G:O6    | 1:XA:1199:U:H2'    | 2.21                     | 0.41              |
| 22:XV:17:C:OP1    | 22:XV:60:U:O2'     | 2.34                     | 0.41              |
| 1:QA:858:G:O6     | 1:QA:869:G:H3'     | 2.20                     | 0.41              |
| 1:QA:598:U:H4'    | 8:QH:94:TYR:CG     | 2.56                     | 0.41              |
| 22:QW:30:G:H2'    | 22:QW:31:G:H8      | 1.85                     | 0.41              |
| 25:RA:307:G:N2    | 25:RA:309:G:H3'    | 2.36                     | 0.41              |
| 41:YV:71:LEU:N    | 41:YV:86:GLY:HA2   | 2.35                     | 0.41              |
| 19:QS:64:GLU:C    | 19:QS:66:MET:H     | 2.22                     | 0.41              |
| 25:YA:590:A:OP1   | 29:YF:95:ARG:NH1   | 2.54                     | 0.41              |
| 47:R1:15:ALA:O    | 47:R1:40:ARG:HG3   | 2.21                     | 0.41              |
| 1:QA:1305:G:OP1   | 21:QU:2:GLY:HA2    | 2.21                     | 0.41              |
| 1:QA:1226:C:OP2   | 13:QM:103:THR:OG1  | 2.30                     | 0.41              |
| 30:YG:38:VAL:HG13 | 30:YG:158:ALA:HB3  | 2.03                     | 0.41              |
| 11:QK:110:ASP:HB3 | 18:QR:85:LEU:HG    | 2.02                     | 0.41              |
| 4:XD:199:ASN:ND2  | 4:XD:199:ASN:O     | 2.37                     | 0.41              |
| 29:RF:125:LEU:N   | 29:RF:125:LEU:HD23 | 2.36                     | 0.41              |
| 1:QA:1301:U:O4    | 1:QA:1303:C:C2     | 2.73                     | 0.41              |
| 14:QN:10:ALA:HB2  | 14:QN:23:ARG:HE    | 1.84                     | 0.41              |
| 25:RA:752:A:H4'   | 25:RA:753:C:O5'    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:775:G:C4    | 25:RA:794:G:C8     | 3.09                     | 0.41              |
| 25:RA:1863:G:H2'  | 25:RA:1864:U:O4'   | 2.20                     | 0.41              |
| 41:YV:28:GLU:HA   | 41:YV:29:PRO:HD3   | 1.88                     | 0.41              |
| 41:RV:64:HIS:CE1  | 41:RV:92:THR:OG1   | 2.74                     | 0.41              |
| 38:RS:106:ARG:HB3 | 38:RS:110:LEU:HD21 | 2.03                     | 0.41              |
| 25:YA:2177:C:H2'  | 25:YA:2178:C:C6    | 2.56                     | 0.41              |
| 3:XC:206:GLU:HB3  | 3:XC:207:VAL:H     | 1.64                     | 0.41              |
| 30:YG:105:LYS:NZ  | 50:Y4:26:SER:HB3   | 2.35                     | 0.41              |
| 48:R2:44:LEU:HA   | 48:R2:44:LEU:HD23  | 1.93                     | 0.41              |
| 25:RA:1105:U:H2'  | 25:RA:1106:G:C8    | 2.55                     | 0.41              |
| 25:YA:2327:A:H2'  | 25:YA:2328:A:C8    | 2.55                     | 0.41              |
| 25:YA:256:A:H2'   | 25:YA:257:A:C8     | 2.56                     | 0.41              |
| 25:RA:2142:C:H2'  | 25:RA:2143:C:C6    | 2.56                     | 0.41              |
| 25:RA:1306:C:H2'  | 25:RA:1307:A:H8    | 1.85                     | 0.41              |
| 25:RA:121:G:H4'   | 25:RA:149:A:H5'    | 2.02                     | 0.41              |
| 2:QB:228:GLY:O    | 2:QB:230:VAL:HG23  | 2.21                     | 0.41              |
| 41:YV:44:LYS:O    | 41:YV:46:VAL:N     | 2.54                     | 0.41              |
| 29:RF:195:ASP:OD1 | 29:RF:196:LEU:N    | 2.54                     | 0.41              |
| 25:RA:2636:U:H2'  | 25:RA:2637:U:H6    | 1.86                     | 0.41              |
| 41:YV:33:VAL:N    | 41:YV:59:ALA:O     | 2.54                     | 0.41              |
| 25:YA:2086:U:H2'  | 25:YA:2087:G:C8    | 2.55                     | 0.41              |
| 33:RN:111:PRO:HA  | 33:RN:114:ARG:NH1  | 2.35                     | 0.41              |
| 8:XH:49:GLU:HG2   | 8:XH:62:TYR:HE2    | 1.85                     | 0.41              |
| 23:XX:22:U:H6     | 23:XX:22:U:H5''    | 1.86                     | 0.41              |
| 31:RH:155:SER:OG  | 31:RH:155:SER:O    | 2.19                     | 0.41              |
| 47:R1:81:LYS:HE3  | 47:R1:81:LYS:HB3   | 1.51                     | 0.41              |
| 25:YA:524:U:H2'   | 25:YA:525:U:C6     | 2.56                     | 0.41              |
| 31:YH:109:PHE:CG  | 31:YH:110:SER:N    | 2.88                     | 0.41              |
| 1:XA:1486:G:H2'   | 1:XA:1487:G:O4'    | 2.21                     | 0.41              |
| 1:QA:1104:G:O3'   | 2:QB:111:ARG:NH2   | 2.53                     | 0.41              |
| 35:RP:59:LEU:CD2  | 54:R8:59:LYS:HE3   | 2.50                     | 0.41              |
| 19:QS:36:ARG:CZ   | 19:QS:73:GLU:HB2   | 2.51                     | 0.41              |
| 1:XA:1392:G:H21   | 1:XA:1502:A:H8     | 1.67                     | 0.41              |
| 25:RA:1688:U:H5'  | 25:RA:1689:A:OP1   | 2.21                     | 0.41              |
| 25:RA:1006:C:C2   | 25:RA:1138:G:N2    | 2.89                     | 0.41              |
| 25:YA:1006:C:O2   | 33:YN:106:MET:HG2  | 2.21                     | 0.41              |
| 27:YD:27:THR:C    | 27:YD:29:PRO:HD2   | 2.40                     | 0.41              |
| 39:RT:118:ARG:HA  | 39:RT:121:ILE:HD12 | 2.02                     | 0.41              |
| 3:QC:186:PHE:HA   | 3:QC:198:VAL:O     | 2.21                     | 0.41              |
| 27:RD:35:LYS:HD2  | 27:RD:104:TYR:CD1  | 2.56                     | 0.41              |
| 35:YP:1:MET:HE1   | 35:YP:6:LEU:HD13   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:990:A:N6    | 25:RA:1186:G:H1'   | 2.36                     | 0.41              |
| 27:RD:71:ASP:OD2  | 27:RD:103:ARG:NH2  | 2.52                     | 0.41              |
| 25:RA:373:U:H2'   | 25:RA:374:A:O5'    | 2.21                     | 0.41              |
| 30:RG:47:LYS:HE3  | 30:RG:47:LYS:HB2   | 1.91                     | 0.41              |
| 25:RA:1151:G:H5'' | 40:RU:81:HIS:NE2   | 2.36                     | 0.41              |
| 1:XA:309:G:H1'    | 1:XA:608:A:C2      | 2.55                     | 0.41              |
| 25:RA:2654:A:H1'  | 25:RA:2656:U:C2    | 2.56                     | 0.41              |
| 25:YA:586:A:H5'   | 29:YF:89:VAL:HG21  | 2.03                     | 0.41              |
| 25:YA:2745:C:H1'  | 31:YH:143:GLN:HG2  | 2.03                     | 0.41              |
| 25:YA:835:A:N6    | 25:YA:836:G:C6     | 2.89                     | 0.41              |
| 25:RA:1796:U:O2'  | 27:RD:256:GLY:N    | 2.53                     | 0.41              |
| 25:RA:1424:G:OP1  | 27:RD:33:LEU:HD12  | 2.20                     | 0.41              |
| 25:RA:220:G:O2'   | 25:RA:233:A:N3     | 2.42                     | 0.41              |
| 1:XA:764:C:H2'    | 1:XA:765:G:O4'     | 2.21                     | 0.41              |
| 1:XA:731:G:H5'    | 1:XA:766:A:H4'     | 2.02                     | 0.41              |
| 25:RA:1854:A:H62  | 25:RA:1888:G:H8    | 1.68                     | 0.41              |
| 25:RA:1857:G:C6   | 25:RA:1858:G:N1    | 2.89                     | 0.41              |
| 25:RA:587:C:N3    | 35:RP:33:ARG:NH1   | 2.68                     | 0.41              |
| 31:YH:30:LYS:HB3  | 31:YH:136:ILE:HG21 | 2.02                     | 0.41              |
| 25:RA:1877:A:H3'  | 25:RA:1878:G:O4'   | 2.21                     | 0.41              |
| 1:QA:1241:G:H2'   | 1:QA:1242:C:C6     | 2.56                     | 0.41              |
| 9:XI:48:GLU:N     | 9:XI:49:PRO:HD2    | 2.35                     | 0.41              |
| 25:RA:2441:C:OP2  | 25:RA:2586:C:O2'   | 2.38                     | 0.41              |
| 1:XA:15:G:C4      | 1:XA:16:A:C8       | 3.08                     | 0.41              |
| 42:YW:4:LYS:HB3   | 42:YW:106:ILE:HG22 | 2.03                     | 0.41              |
| 25:RA:277:C:H5''  | 25:RA:278:A:C8     | 2.55                     | 0.41              |
| 25:YA:2565:A:H5'' | 25:YA:2566:A:OP2   | 2.21                     | 0.41              |
| 2:XB:37:ASN:O     | 2:XB:37:ASN:ND2    | 2.47                     | 0.41              |
| 2:QB:156:LYS:HD2  | 2:QB:156:LYS:HA    | 1.92                     | 0.41              |
| 17:QQ:52:LYS:HE3  | 17:QQ:52:LYS:HB3   | 1.81                     | 0.41              |
| 4:XD:149:ALA:O    | 4:XD:153:ARG:HG2   | 2.21                     | 0.41              |
| 6:XF:91:VAL:HG12  | 6:XF:92:LYS:O      | 2.21                     | 0.41              |
| 31:RH:80:SER:OG   | 31:RH:81:GLU:N     | 2.53                     | 0.41              |
| 44:RY:101:LYS:HE3 | 44:RY:101:LYS:HB3  | 1.93                     | 0.41              |
| 44:YY:96:ILE:HG12 | 44:YY:101:LYS:HG3  | 2.03                     | 0.41              |
| 1:QA:1347:G:O2'   | 1:QA:1348:U:P      | 2.79                     | 0.41              |
| 1:QA:1320:C:C4    | 19:QS:36:ARG:HG2   | 2.56                     | 0.41              |
| 1:QA:1399:C:H4'   | 1:QA:1400:C:H5''   | 2.02                     | 0.41              |
| 4:XD:9:CYS:SG     | 4:XD:26:CYS:SG     | 3.19                     | 0.41              |
| 44:YY:15:VAL:HG12 | 44:YY:17:SER:OG    | 2.21                     | 0.41              |
| 19:XS:12:ASP:H    | 19:XS:38:SER:HB3   | 1.86                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:1980:G:N3   | 25:RA:1982:C:C5    | 2.88                     | 0.41              |
| 47:Y1:85:LEU:HD23 | 47:Y1:85:LEU:HA    | 1.90                     | 0.41              |
| 25:YA:1300:U:H4'  | 25:YA:1301:A:O5'   | 2.20                     | 0.41              |
| 25:YA:2439:A:P    | 25:YA:2439:A:H3'   | 2.61                     | 0.41              |
| 25:YA:2439:A:H4'  | 25:YA:2440:C:O5'   | 2.21                     | 0.41              |
| 21:XU:8:THR:HB    | 21:XU:11:GLY:H     | 1.86                     | 0.41              |
| 33:YN:34:LEU:HD11 | 33:YN:120:LEU:HB2  | 2.02                     | 0.41              |
| 25:YA:1816:G:N7   | 27:YD:62:TYR:CE1   | 2.89                     | 0.41              |
| 31:RH:3:ARG:HD3   | 31:RH:6:ARG:HH21   | 1.85                     | 0.41              |
| 19:XS:62:ILE:HA   | 19:XS:66:MET:HE1   | 2.02                     | 0.41              |
| 25:RA:1328:G:H2'  | 25:RA:1330:C:C5    | 2.56                     | 0.41              |
| 25:RA:1330:C:H2'  | 25:RA:1331:A:C8    | 2.52                     | 0.41              |
| 1:QA:1288:A:H2'   | 1:QA:1289:A:C8     | 2.55                     | 0.41              |
| 25:RA:139:G:C6    | 25:RA:140:G:H2'    | 2.56                     | 0.41              |
| 35:YP:6:LEU:HD13  | 35:YP:6:LEU:HA     | 1.78                     | 0.41              |
| 35:RP:45:LEU:HA   | 35:RP:45:LEU:HD12  | 1.83                     | 0.41              |
| 25:YA:2314:C:H2'  | 25:YA:2315:G:C8    | 2.56                     | 0.41              |
| 25:YA:2314:C:H5'' | 30:YG:38:VAL:HG11  | 2.02                     | 0.41              |
| 25:RA:1264:G:H5'  | 51:R5:11:THR:CG2   | 2.51                     | 0.41              |
| 3:XC:23:TYR:HE1   | 10:XJ:92:THR:HG23  | 1.86                     | 0.41              |
| 26:YB:24:G:H5''   | 26:YB:25:A:OP1     | 2.21                     | 0.41              |
| 31:RH:86:GLU:H    | 31:RH:86:GLU:CD    | 2.24                     | 0.41              |
| 31:RH:89:ILE:HD11 | 31:RH:129:THR:HG22 | 2.03                     | 0.41              |
| 1:XA:1033:G:H2'   | 1:XA:1034:G:C8     | 2.56                     | 0.41              |
| 25:RA:2127:G:O2'  | 25:RA:2173:A:N1    | 2.38                     | 0.41              |
| 25:RA:2661:G:H2'  | 25:RA:2662:A:O4'   | 2.20                     | 0.41              |
| 30:RG:38:VAL:HG13 | 30:RG:158:ALA:HB3  | 2.03                     | 0.41              |
| 20:QT:104:LEU:HB3 | 20:QT:105:SER:H    | 1.51                     | 0.41              |
| 1:QA:1065:U:P     | 1:QA:1190:G:H22    | 2.43                     | 0.41              |
| 28:YE:36:ARG:HH21 | 28:YE:88:GLY:CA    | 2.32                     | 0.41              |
| 3:QC:134:ILE:HG22 | 3:QC:168:ALA:HB3   | 2.02                     | 0.41              |
| 25:RA:334:C:OP1   | 25:RA:335:C:N4     | 2.52                     | 0.41              |
| 41:YV:61:VAL:O    | 41:YV:63:GLY:N     | 2.54                     | 0.41              |
| 22:QV:50:U:H2'    | 22:QV:51:C:H6      | 1.86                     | 0.41              |
| 50:Y4:46:GLN:NE2  | 50:Y4:48:ARG:HD3   | 2.36                     | 0.41              |
| 1:QA:224:C:H2'    | 1:QA:225:C:H6      | 1.86                     | 0.41              |
| 11:XK:120:ARG:HA  | 11:XK:121:PRO:HD3  | 1.86                     | 0.41              |
| 3:QC:174:PRO:O    | 3:QC:177:THR:HG22  | 2.21                     | 0.41              |
| 1:QA:269:C:H2'    | 1:QA:270:A:H8      | 1.84                     | 0.41              |
| 50:Y4:26:SER:OG   | 50:Y4:27:THR:N     | 2.50                     | 0.41              |
| 25:YA:500:G:N2    | 25:YA:502:A:H3'    | 2.36                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:QA:834:C:H2'     | 1:QA:835:U:C6     | 2.56                     | 0.41              |
| 31:YH:59:ARG:C     | 31:YH:61:HIS:H    | 2.23                     | 0.41              |
| 25:RA:725:G:C6     | 25:RA:726:G:N1    | 2.88                     | 0.41              |
| 25:RA:1357:U:H2'   | 25:RA:1358:G:O4'  | 2.20                     | 0.41              |
| 25:RA:1877:A:H5'   | 25:RA:1878:G:OP2  | 2.21                     | 0.41              |
| 48:R2:32:LEU:HD21  | 48:R2:54:LYS:HG2  | 2.03                     | 0.41              |
| 25:RA:311:A:C6     | 25:RA:328:U:C4    | 3.09                     | 0.41              |
| 1:QA:993:G:O6      | 1:QA:1045:C:N4    | 2.44                     | 0.41              |
| 1:QA:742:G:H2'     | 1:QA:743:U:O4'    | 2.20                     | 0.41              |
| 2:QB:16:HIS:HB2    | 2:QB:17:PHE:CD2   | 2.55                     | 0.41              |
| 8:XH:38:ILE:HD12   | 8:XH:118:VAL:HG12 | 2.02                     | 0.41              |
| 25:YA:1338:G:N7    | 43:YX:62:LYS:NZ   | 2.50                     | 0.41              |
| 7:QG:115:ARG:O     | 7:QG:118:VAL:HG22 | 2.21                     | 0.41              |
| 5:XE:127:ASN:HA    | 5:XE:128:PRO:HD3  | 1.93                     | 0.41              |
| 1:QA:639:G:H2'     | 1:QA:640:A:H8     | 1.85                     | 0.41              |
| 27:RD:261:LYS:HB2  | 27:RD:261:LYS:HE3 | 1.91                     | 0.41              |
| 9:XI:53:VAL:HG13   | 9:XI:95:LYS:HE3   | 2.03                     | 0.41              |
| 7:QG:94:ARG:NH1    | 7:QG:98:SER:OG    | 2.54                     | 0.41              |
| 1:XA:204:U:O2'     | 1:XA:216:G:O4'    | 2.37                     | 0.41              |
| 4:XD:39:PRO:HA     | 4:XD:40:PRO:HD3   | 1.90                     | 0.41              |
| 39:RT:60:THR:HG22  | 39:RT:77:PRO:HA   | 2.02                     | 0.41              |
| 37:YR:67:LEU:HD13  | 37:YR:76:VAL:HG21 | 2.03                     | 0.41              |
| 11:QK:93:GLN:OE1   | 11:QK:96:ARG:NH1  | 2.54                     | 0.41              |
| 50:R4:46:GLN:HE21  | 50:R4:48:ARG:HD3  | 1.85                     | 0.41              |
| 20:XT:97:ALA:O     | 20:XT:99:LEU:N    | 2.53                     | 0.41              |
| 39:YT:11:GLU:N     | 39:YT:11:GLU:OE1  | 2.53                     | 0.41              |
| 26:RB:24:G:H5''    | 26:RB:25:A:OP1    | 2.21                     | 0.41              |
| 1:QA:398:C:H2'     | 1:QA:399:G:C8     | 2.56                     | 0.41              |
| 48:R2:16:LEU:O     | 48:R2:20:GLU:HB2  | 2.21                     | 0.41              |
| 25:YA:253:C:H2'    | 25:YA:254:G:O4'   | 2.21                     | 0.41              |
| 27:YD:142:VAL:HG12 | 27:YD:163:ALA:HB3 | 2.03                     | 0.41              |
| 25:RA:2702:U:OP1   | 25:RA:2702:U:H6   | 2.03                     | 0.41              |
| 31:YH:9:ILE:HB     | 31:YH:10:PRO:CA   | 2.50                     | 0.41              |
| 1:XA:1493:A:C3'    | 1:XA:1494:G:H5'   | 2.51                     | 0.41              |
| 41:YV:35:LEU:HD23  | 41:YV:37:VAL:HG21 | 2.03                     | 0.41              |
| 1:QA:350:G:C2'     | 1:QA:351:G:H5'    | 2.51                     | 0.41              |
| 47:R1:58:ILE:HG23  | 47:R1:87:PRO:HG3  | 2.03                     | 0.41              |
| 25:YA:2029:G:H2'   | 25:YA:2031:A:OP1  | 2.21                     | 0.41              |
| 25:RA:394:A:N1     | 25:RA:395:U:N3    | 2.68                     | 0.41              |
| 52:Y6:12:GLU:CD    | 52:Y6:12:GLU:H    | 2.25                     | 0.41              |
| 32:YI:122:GLU:HB3  | 32:YI:126:TYR:OH  | 2.21                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:XI:20:ARG:HA     | 9:XI:21:PRO:HD3   | 1.85                     | 0.41              |
| 25:RA:559:G:N2     | 40:RU:49:HIS:CE1  | 2.88                     | 0.41              |
| 48:Y2:21:LEU:HA    | 48:Y2:21:LEU:HD23 | 1.82                     | 0.41              |
| 25:RA:877:U:O2'    | 25:RA:878:A:OP1   | 2.35                     | 0.41              |
| 20:XT:104:LEU:HB3  | 20:XT:105:SER:H   | 1.53                     | 0.41              |
| 25:RA:1971:A:C4    | 27:RD:241:PRO:HD3 | 2.55                     | 0.41              |
| 25:RA:923:C:H2'    | 25:RA:924:C:C6    | 2.55                     | 0.41              |
| 25:YA:2148:G:H2'   | 25:YA:2149:G:H8   | 1.86                     | 0.41              |
| 1:XA:512:U:H2'     | 1:XA:513:C:H6     | 1.86                     | 0.41              |
| 1:QA:1118:C:H1'    | 1:QA:1179:A:C5    | 2.56                     | 0.41              |
| 22:XW:63:G:H2'     | 22:XW:64:G:C8     | 2.56                     | 0.41              |
| 41:RV:38:LEU:HD21  | 41:RV:57:VAL:HG23 | 2.03                     | 0.41              |
| 1:QA:706:A:O4'     | 11:QK:29:ILE:HD11 | 2.21                     | 0.41              |
| 29:RF:140:LEU:HD12 | 29:RF:140:LEU:HA  | 1.78                     | 0.41              |
| 25:RA:2018:G:H2'   | 25:RA:2019:A:C8   | 2.56                     | 0.41              |
| 1:QA:512:U:H2'     | 1:QA:513:C:H6     | 1.86                     | 0.41              |
| 1:XA:939:G:H2'     | 1:XA:940:C:C6     | 2.56                     | 0.41              |
| 1:XA:922:G:H2'     | 1:XA:923:A:C8     | 2.57                     | 0.41              |
| 3:QC:68:VAL:HG12   | 3:QC:70:VAL:HG23  | 2.03                     | 0.41              |
| 25:RA:2075:U:C4    | 25:RA:2238:G:C6   | 3.09                     | 0.41              |
| 20:XT:65:LYS:O     | 20:XT:68:LYS:HG2  | 2.21                     | 0.41              |
| 25:RA:2065:C:H1'   | 25:RA:2449:U:O2   | 2.21                     | 0.41              |
| 25:RA:1384:A:N3    | 25:RA:1405:U:H1'  | 2.36                     | 0.41              |
| 1:QA:1186:G:N2     | 14:QN:61:TRP:O    | 2.44                     | 0.41              |
| 1:XA:189(D):C:O2   | 1:XA:189(H):G:N1  | 2.54                     | 0.41              |
| 42:RW:9:TYR:H      | 42:RW:102:HIS:CE1 | 2.39                     | 0.41              |
| 25:RA:2839:G:H5'   | 37:RR:46:GLY:HA2  | 2.03                     | 0.41              |
| 13:QM:9:ILE:HG12   | 13:QM:9:ILE:H     | 1.60                     | 0.41              |
| 25:YA:432:A:H2'    | 25:YA:433:C:C6    | 2.56                     | 0.41              |
| 27:YD:224:ALA:HA   | 27:YD:233:HIS:O   | 2.21                     | 0.41              |
| 40:RU:37:GLU:HA    | 40:RU:40:PHE:CD1  | 2.56                     | 0.41              |
| 25:RA:1224:C:O3'   | 41:RV:85:LYS:HD3  | 2.21                     | 0.40              |
| 1:QA:1382:C:O2'    | 22:QW:34:C:OP1    | 2.36                     | 0.40              |
| 25:YA:826:U:H4'    | 35:YP:55:ARG:HA   | 2.03                     | 0.40              |
| 25:RA:1980:G:C2    | 25:RA:1982:C:C4   | 3.09                     | 0.40              |
| 25:YA:60:G:C2      | 25:YA:74:A:C5     | 3.10                     | 0.40              |
| 1:XA:1318:A:H4'    | 19:XS:10:PHE:CE2  | 2.56                     | 0.40              |
| 31:YH:35:VAL:HG11  | 31:YH:72:ILE:HG13 | 2.03                     | 0.40              |
| 25:YA:320:A:H4'    | 25:YA:322:A:N7    | 2.35                     | 0.40              |
| 25:YA:1639:U:C2'   | 25:YA:1640:C:H5'' | 2.49                     | 0.40              |
| 25:RA:2208:A:H1'   | 25:RA:2219:G:C5   | 2.55                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:R3:8:LEU:CD1   | 49:R3:31:LEU:HD12  | 2.51                     | 0.40              |
| 2:XB:25:ASN:C     | 2:XB:27:LYS:H      | 2.24                     | 0.40              |
| 28:YE:52:LEU:HB3  | 28:YE:75:VAL:HG23  | 2.03                     | 0.40              |
| 2:XB:221:LEU:HA   | 2:XB:224:GLN:HB2   | 2.02                     | 0.40              |
| 25:RA:576:U:H4'   | 25:RA:2502:G:C8    | 2.57                     | 0.40              |
| 25:RA:2292:C:P    | 38:RS:17:ARG:HH22  | 2.44                     | 0.40              |
| 1:QA:1237:C:C4    | 1:QA:1336:C:O2     | 2.74                     | 0.40              |
| 25:YA:2159:G:H2'  | 25:YA:2160:G:C8    | 2.56                     | 0.40              |
| 5:XE:7:GLU:HB3    | 5:XE:35:GLY:O      | 2.21                     | 0.40              |
| 1:QA:254:G:OP1    | 17:QQ:66:SER:OG    | 2.31                     | 0.40              |
| 34:YO:71:ARG:NE   | 34:YO:105:GLU:OE2  | 2.55                     | 0.40              |
| 18:XR:22:VAL:HG13 | 18:XR:23:LYS:N     | 2.36                     | 0.40              |
| 25:YA:1140:C:H2'  | 25:YA:1141:U:H5'   | 2.03                     | 0.40              |
| 28:RE:117:MET:HG3 | 28:RE:122:PHE:O    | 2.20                     | 0.40              |
| 41:YV:77:ALA:O    | 41:YV:79:VAL:HG22  | 2.21                     | 0.40              |
| 11:QK:44:SER:O    | 11:QK:48:ILE:HG12  | 2.21                     | 0.40              |
| 25:YA:1425:G:N1   | 25:YA:1426:G:C2    | 2.89                     | 0.40              |
| 25:YA:2395:C:H2'  | 25:YA:2396:G:O4'   | 2.21                     | 0.40              |
| 13:XM:40:ASN:HB3  | 13:XM:43:THR:HG23  | 2.04                     | 0.40              |
| 1:XA:1140:C:H2'   | 1:XA:1141:C:H6     | 1.86                     | 0.40              |
| 1:XA:751:U:H4'    | 15:XO:24:SER:HA    | 2.02                     | 0.40              |
| 28:RE:54:GLN:HB2  | 28:RE:55:ASN:H     | 1.68                     | 0.40              |
| 25:RA:2146:C:H4'  | 25:RA:2147:G:O4'   | 2.21                     | 0.40              |
| 11:XK:62:GLN:OE1  | 11:XK:93:GLN:NE2   | 2.54                     | 0.40              |
| 25:YA:1668:A:H4'  | 25:YA:1669:A:O5'   | 2.21                     | 0.40              |
| 1:XA:270:A:C5     | 1:XA:271:C:C4      | 3.09                     | 0.40              |
| 22:QW:53:G:H1     | 22:QW:61:C:H42     | 1.68                     | 0.40              |
| 40:RU:58:ARG:HA   | 40:RU:61:TRP:CE3   | 2.56                     | 0.40              |
| 42:RW:47:VAL:HA   | 42:RW:50:VAL:HG12  | 2.04                     | 0.40              |
| 25:YA:1525:G:H2'  | 25:YA:1526:G:H8    | 1.86                     | 0.40              |
| 41:RV:62:LEU:HB3  | 41:RV:93:GLU:O     | 2.21                     | 0.40              |
| 49:Y3:46:ASN:O    | 49:Y3:50:VAL:HG22  | 2.21                     | 0.40              |
| 25:YA:2816:C:O2   | 25:YA:2883:A:O2'   | 2.33                     | 0.40              |
| 34:YO:4:PRO:O     | 34:YO:5:GLN:HB2    | 2.21                     | 0.40              |
| 30:RG:97:ASP:O    | 30:RG:101:ILE:HG23 | 2.22                     | 0.40              |
| 4:QD:108:LEU:HD12 | 4:QD:108:LEU:HA    | 1.77                     | 0.40              |
| 45:RZ:148:ASP:N   | 45:RZ:148:ASP:OD2  | 2.53                     | 0.40              |
| 25:RA:2676:C:OP1  | 34:RO:31:LYS:NZ    | 2.50                     | 0.40              |
| 3:XC:174:PRO:O    | 3:XC:177:THR:HG22  | 2.21                     | 0.40              |
| 15:XO:75:PRO:HB2  | 15:XO:79:ARG:HH21  | 1.86                     | 0.40              |
| 1:QA:1031:G:H2'   | 1:QA:1032:G:C8     | 2.57                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:RA:2748:A:H8   | 31:RH:63:SER:CB    | 2.33                     | 0.40              |
| 1:QA:1493:A:O2'   | 24:QY:55:PRO:HD2   | 2.22                     | 0.40              |
| 25:RA:329:G:N7    | 44:RY:19:LYS:HE2   | 2.36                     | 0.40              |
| 22:QV:3:C:H2'     | 22:QV:3:C:O2       | 2.21                     | 0.40              |
| 25:RA:1025:G:C4   | 25:RA:1135:C:H1'   | 2.57                     | 0.40              |
| 25:YA:2030:A:H4'  | 25:YA:2031:A:H8    | 1.86                     | 0.40              |
| 42:RW:92:ARG:NH1  | 42:RW:94:ASP:OD2   | 2.54                     | 0.40              |
| 21:QU:7:ARG:HB3   | 21:QU:21:TYR:CE2   | 2.57                     | 0.40              |
| 1:QA:1300:G:H1'   | 1:QA:1301:U:H5     | 1.85                     | 0.40              |
| 1:XA:1036:G:H5'   | 1:XA:1037:C:C5     | 2.56                     | 0.40              |
| 8:QH:20:TYR:HE2   | 8:QH:75:ARG:HD2    | 1.86                     | 0.40              |
| 25:YA:250:G:C6    | 25:YA:251:A:C6     | 3.09                     | 0.40              |
| 26:RB:79:C:H2'    | 26:RB:80:U:H5'     | 2.02                     | 0.40              |
| 1:QA:1432:G:OP1   | 39:RT:107:ASP:HB2  | 2.20                     | 0.40              |
| 1:XA:336:C:H2'    | 1:XA:337:C:C6      | 2.56                     | 0.40              |
| 15:QO:21:ASP:OD2  | 15:QO:24:SER:HB2   | 2.21                     | 0.40              |
| 10:QJ:54:PHE:HE1  | 10:QJ:55:LYS:HZ2   | 1.68                     | 0.40              |
| 30:RG:143:GLU:OE1 | 30:RG:143:GLU:N    | 2.50                     | 0.40              |
| 36:YQ:80:GLU:HG2  | 36:YQ:81:VAL:N     | 2.35                     | 0.40              |
| 33:YN:43:THR:HB   | 33:YN:46:VAL:HG12  | 2.03                     | 0.40              |
| 3:XC:68:VAL:HG12  | 3:XC:70:VAL:HG23   | 2.03                     | 0.40              |
| 25:RA:222:A:C6    | 25:RA:224:G:C2     | 3.10                     | 0.40              |
| 28:RE:4:ILE:HG21  | 28:RE:92:THR:O     | 2.22                     | 0.40              |
| 25:YA:1814:G:H4'  | 27:YD:51:VAL:HG21  | 2.03                     | 0.40              |
| 28:YE:105:THR:HB  | 28:YE:197:ILE:HG12 | 2.03                     | 0.40              |
| 29:RF:10:PRO:HA   | 29:RF:127:GLU:HB3  | 2.03                     | 0.40              |
| 31:RH:90:LYS:HE2  | 31:RH:90:LYS:HB3   | 1.91                     | 0.40              |
| 11:XK:127:LYS:HD3 | 11:XK:127:LYS:HA   | 1.92                     | 0.40              |
| 50:Y4:2:LYS:HE3   | 50:Y4:2:LYS:HB2    | 1.84                     | 0.40              |
| 25:RA:739:G:N2    | 25:RA:740:U:O4     | 2.44                     | 0.40              |
| 18:XR:66:LEU:O    | 18:XR:70:ILE:HG13  | 2.21                     | 0.40              |
| 44:RY:84:ARG:O    | 44:RY:84:ARG:HG3   | 2.22                     | 0.40              |
| 50:R4:58:ARG:NH2  | 50:R4:62:ARG:HG3   | 2.36                     | 0.40              |
| 35:RP:47:ASP:OD1  | 35:RP:50:ARG:NH1   | 2.55                     | 0.40              |
| 30:YG:82:LEU:HA   | 30:YG:86:MET:SD    | 2.62                     | 0.40              |
| 25:YA:662:G:OP1   | 35:YP:15:ARG:NH2   | 2.55                     | 0.40              |
| 31:RH:156:ALA:HB3 | 31:RH:159:GLU:O    | 2.21                     | 0.40              |
| 2:QB:29:ALA:HB1   | 2:QB:30:ARG:NH2    | 2.32                     | 0.40              |
| 19:XS:29:ARG:HB2  | 19:XS:48:THR:OG1   | 2.22                     | 0.40              |
| 35:YP:83:VAL:CG1  | 35:YP:112:LEU:HD21 | 2.50                     | 0.40              |
| 25:YA:910:A:C6    | 25:YA:911:A:C6     | 3.08                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:QF:69:GLU:O      | 6:QF:72:VAL:HG12   | 2.21                     | 0.40              |
| 25:RA:576:U:H6     | 25:RA:576:U:O5'    | 2.05                     | 0.40              |
| 39:RT:6:LEU:O      | 39:RT:10:VAL:HG23  | 2.21                     | 0.40              |
| 31:RH:108:GLY:HA3  | 31:RH:152:ARG:NH2  | 2.36                     | 0.40              |
| 1:XA:1029:C:O2     | 1:XA:1033:G:N2     | 2.54                     | 0.40              |
| 1:QA:560:U:H4'     | 1:QA:561:U:C5'     | 2.50                     | 0.40              |
| 20:XT:17:ARG:HA    | 20:XT:20:LEU:HD12  | 2.03                     | 0.40              |
| 25:YA:137(A):G:H2' | 25:YA:139:G:N7     | 2.37                     | 0.40              |
| 1:XA:482:A:H5'     | 1:XA:483:C:OP2     | 2.21                     | 0.40              |
| 1:QA:513:C:H2'     | 1:QA:514:C:C6      | 2.56                     | 0.40              |
| 50:Y4:26:SER:HG    | 50:Y4:27:THR:N     | 2.19                     | 0.40              |
| 47:R1:88:LYS:O     | 47:R1:91:LYS:HB2   | 2.21                     | 0.40              |
| 38:RS:74:ALA:HB1   | 38:RS:107:GLU:CB   | 2.50                     | 0.40              |
| 3:QC:69:HIS:HA     | 3:QC:104:GLN:HB2   | 2.03                     | 0.40              |
| 2:QB:121:LEU:HA    | 2:QB:124:SER:HB3   | 2.04                     | 0.40              |
| 25:RA:2243:U:O2'   | 25:RA:2244:U:H5'   | 2.21                     | 0.40              |
| 42:YW:71:VAL:HA    | 42:YW:107:LEU:HD12 | 2.03                     | 0.40              |
| 3:QC:86:VAL:O      | 3:QC:90:GLU:N      | 2.55                     | 0.40              |
| 45:YZ:156:LYS:HB3  | 45:YZ:157:LEU:H    | 1.63                     | 0.40              |
| 45:YZ:158:PRO:HB2  | 45:YZ:161:VAL:HG23 | 2.03                     | 0.40              |
| 25:YA:2533:A:H2'   | 25:YA:2534:A:O4'   | 2.20                     | 0.40              |
| 25:RA:1600:C:H1'   | 53:R7:49:ARG:HH21  | 1.85                     | 0.40              |
| 1:QA:35:G:H2'      | 1:QA:36:C:C6       | 2.56                     | 0.40              |
| 31:RH:33:LEU:HA    | 31:RH:33:LEU:HD12  | 1.96                     | 0.40              |
| 40:YU:17:ILE:HG23  | 40:YU:39:LEU:HD12  | 2.03                     | 0.40              |
| 25:RA:2870:C:H2'   | 25:RA:2871:C:O4'   | 2.21                     | 0.40              |
| 25:RA:1843:C:H5'   | 27:RD:253:GLN:OE1  | 2.21                     | 0.40              |
| 25:YA:588:U:H1'    | 29:YF:90:PHE:HB3   | 2.03                     | 0.40              |
| 32:YI:72:LEU:HD21  | 32:YI:107:VAL:HG11 | 2.03                     | 0.40              |
| 28:RE:35:GLN:HE22  | 28:RE:37:ARG:HH21  | 1.69                     | 0.40              |
| 24:XY:54:HIS:HA    | 24:XY:55:PRO:HD3   | 1.91                     | 0.40              |
| 44:YY:17:SER:CB    | 44:YY:71:LYS:HB3   | 2.50                     | 0.40              |
| 19:XS:39:THR:HA    | 19:XS:70:LYS:HA    | 2.02                     | 0.40              |
| 50:R4:58:ARG:HG3   | 50:R4:59:PHE:N     | 2.37                     | 0.40              |
| 25:YA:2564:A:C2    | 25:YA:2647:U:H4'   | 2.57                     | 0.40              |
| 19:QS:63:THR:H     | 19:QS:66:MET:CE    | 2.34                     | 0.40              |
| 26:YB:81:G:H5'     | 26:YB:81:G:N3      | 2.36                     | 0.40              |
| 1:XA:316:G:C2      | 1:XA:317:G:N7      | 2.90                     | 0.40              |
| 25:RA:2750:A:OP2   | 31:RH:6:ARG:NH2    | 2.54                     | 0.40              |
| 25:RA:2849:U:H2'   | 25:RA:2866:U:O2    | 2.21                     | 0.40              |
| 25:RA:1568:G:P     | 27:RD:63:ARG:HH12  | 2.44                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:YP:45:LEU:HD22  | 35:YP:45:LEU:HA    | 1.78                     | 0.40              |
| 25:RA:140:G:H1'    | 25:RA:141:A:C2     | 2.56                     | 0.40              |
| 25:RA:873:G:H1     | 25:RA:904:C:N4     | 2.17                     | 0.40              |
| 12:QL:126:LYS:O    | 12:QL:128:ALA:N    | 2.54                     | 0.40              |
| 4:QD:73:ARG:HD2    | 4:QD:73:ARG:HA     | 1.86                     | 0.40              |
| 45:RZ:69:THR:HG22  | 45:RZ:90:VAL:HG22  | 2.04                     | 0.40              |
| 35:YP:100:LEU:HD23 | 35:YP:100:LEU:HA   | 1.92                     | 0.40              |
| 35:YP:126:VAL:HG22 | 35:YP:145:PRO:HG2  | 2.02                     | 0.40              |
| 25:RA:363(F):A:H1' | 25:RA:364:C:C5     | 2.57                     | 0.40              |
| 27:YD:184:LYS:HE3  | 27:YD:269:PHE:HA   | 2.02                     | 0.40              |
| 1:XA:1068:G:H5'    | 1:XA:1388:C:OP1    | 2.20                     | 0.40              |
| 25:RA:55:G:H2'     | 25:RA:56:A:C8      | 2.56                     | 0.40              |
| 1:QA:1055:A:O2'    | 3:QC:161:GLU:OE2   | 2.26                     | 0.40              |
| 1:QA:6:G:H4'       | 1:QA:298:A:H4'     | 2.02                     | 0.40              |
| 22:XW:71:C:O3'     | 25:YA:1851:U:O2'   | 2.40                     | 0.40              |
| 25:YA:1608:A:H1'   | 25:YA:1610:A:OP2   | 2.21                     | 0.40              |
| 25:RA:1001:A:H2'   | 25:RA:1002:G:O4'   | 2.22                     | 0.40              |
| 27:YD:165:ILE:HD13 | 27:YD:175:LEU:HD21 | 2.02                     | 0.40              |
| 35:RP:30:THR:O     | 35:RP:33:ARG:HB2   | 2.22                     | 0.40              |
| 25:RA:2065:C:O2    | 25:RA:2449:U:N3    | 2.52                     | 0.40              |
| 25:RA:1154:G:OP1   | 40:RU:58:ARG:HD3   | 2.22                     | 0.40              |
| 38:RS:67:ARG:O     | 38:RS:71:ARG:HG3   | 2.21                     | 0.40              |
| 22:XV:31:G:C5      | 22:XV:32:C:C5      | 3.10                     | 0.40              |
| 42:YW:13:SER:HA    | 42:YW:14:PRO:HD3   | 1.87                     | 0.40              |
| 22:XV:47:U:H3'     | 22:XV:48:C:H5'     | 2.03                     | 0.40              |
| 25:RA:2072:G:H2'   | 25:RA:2073:C:O4'   | 2.21                     | 0.40              |
| 25:YA:2600:A:H2'   | 25:YA:2601:C:C6    | 2.57                     | 0.40              |
| 22:XV:62:C:H2'     | 22:XV:63:G:C8      | 2.56                     | 0.40              |
| 25:RA:1792:G:H2'   | 25:RA:1793:C:H6    | 1.87                     | 0.40              |
| 25:RA:885:C:H1'    | 25:RA:890:A:N6     | 2.36                     | 0.40              |
| 25:YA:2817:G:OP1   | 37:YR:99:LYS:HE2   | 2.21                     | 0.40              |
| 25:YA:94:G:H2'     | 25:YA:95:G:O4'     | 2.21                     | 0.40              |
| 25:YA:1329:U:H5''  | 25:YA:1330:C:H5    | 1.86                     | 0.40              |
| 1:XA:710:G:OP1     | 6:XF:54:LYS:HE2    | 2.22                     | 0.40              |
| 5:XE:152:ARG:NH2   | 8:XH:107:LEU:O     | 2.54                     | 0.40              |
| 25:RA:1444:G:H2'   | 25:RA:1445(A):C:C5 | 2.56                     | 0.40              |
| 30:YG:41:GLN:HB3   | 30:YG:43:LEU:HD13  | 2.02                     | 0.40              |
| 45:YZ:182:LYS:HE3  | 45:YZ:182:LYS:HB3  | 1.95                     | 0.40              |
| 4:QD:169:LYS:HE2   | 4:QD:169:LYS:HB3   | 1.85                     | 0.40              |
| 24:QY:79:ILE:HG22  | 24:QY:84:TYR:CE2   | 2.57                     | 0.40              |
| 27:YD:61:LEU:HA    | 27:YD:61:LEU:HD12  | 1.78                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:YF:118:ALA:HB2 | 29:YF:123:LEU:HD22 | 2.03                     | 0.40              |
| 53:Y7:48:LYS:HB2  | 53:Y7:49:ARG:H     | 1.62                     | 0.40              |
| 7:QG:155:ARG:HB3  | 7:QG:156:TRP:H     | 1.54                     | 0.40              |
| 31:YH:116:GLU:HA  | 31:YH:117:PRO:HD3  | 1.90                     | 0.40              |
| 37:RR:70:LEU:C    | 37:RR:72:ASP:H     | 2.23                     | 0.40              |
| 32:YI:76:THR:HG21 | 32:YI:138:ILE:HD11 | 2.02                     | 0.40              |
| 39:YT:55:ASN:H    | 39:YT:59:THR:HG22  | 1.85                     | 0.40              |
| 41:YV:5:VAL:HG11  | 41:YV:14:VAL:HG13  | 2.04                     | 0.40              |
| 25:RA:826:U:H4'   | 35:RP:55:ARG:HA    | 2.04                     | 0.40              |
| 25:YA:2733:A:C2   | 28:YE:203:LYS:HA   | 2.56                     | 0.40              |
| 28:YE:203:LYS:HE3 | 28:YE:203:LYS:HB2  | 1.75                     | 0.40              |
| 1:XA:872:A:C4     | 1:XA:874:G:C8      | 3.09                     | 0.40              |
| 52:R6:40:CYS:N    | 52:R6:41:PRO:HD3   | 2.36                     | 0.40              |
| 25:RA:413:C:H4'   | 25:RA:1880:C:O2'   | 2.22                     | 0.40              |
| 4:QD:111:ALA:HA   | 4:QD:161:ASN:ND2   | 2.37                     | 0.40              |
| 1:QA:148:G:H2'    | 1:QA:149:A:C8      | 2.52                     | 0.40              |
| 1:QA:1237:C:C2'   | 1:QA:1238:A:OP1    | 2.70                     | 0.40              |
| 10:XJ:10:GLY:HA3  | 10:XJ:16:LEU:CD2   | 2.51                     | 0.40              |
| 27:RD:102:LYS:C   | 27:RD:103:ARG:HG2  | 2.41                     | 0.40              |
| 13:XM:44:ARG:C    | 13:XM:46:LYS:H     | 2.25                     | 0.40              |
| 25:YA:2261:C:OP1  | 46:Y0:17:GLN:HB2   | 2.22                     | 0.40              |
| 29:RF:63:LYS:HE2  | 29:RF:67:GLN:HB2   | 2.03                     | 0.40              |
| 25:RA:859:G:C2'   | 25:RA:860:U:OP2    | 2.69                     | 0.40              |
| 25:RA:296:C:H2'   | 25:RA:297:C:H6     | 1.83                     | 0.40              |
| 45:RZ:110:GLY:N   | 45:RZ:142:SER:HB2  | 2.35                     | 0.40              |
| 39:RT:102:ILE:O   | 39:RT:106:SER:HB3  | 2.21                     | 0.40              |
| 25:RA:1914:C:C2'  | 25:RA:1915:U:O5'   | 2.70                     | 0.40              |
| 25:RA:1316:U:H2'  | 25:RA:1317:A:H8    | 1.87                     | 0.40              |
| 1:XA:482:A:H3'    | 1:XA:483:C:C6      | 2.57                     | 0.40              |
| 25:RA:1345:C:H2'  | 25:RA:1346:G:C8    | 2.57                     | 0.40              |
| 32:YI:1:MET:HG3   | 32:YI:23:PRO:HG3   | 2.03                     | 0.40              |
| 1:XA:108:G:H5'    | 1:XA:109:A:H5''    | 2.02                     | 0.40              |
| 25:YA:1418:G:OP1  | 25:YA:1588:C:O2'   | 2.37                     | 0.40              |
| 1:XA:766:A:H2'    | 1:XA:767:A:O4'     | 2.21                     | 0.40              |
| 1:XA:16:A:N1      | 1:XA:919:A:H2      | 2.19                     | 0.40              |
| 30:YG:41:GLN:HG2  | 30:YG:154:GLY:O    | 2.21                     | 0.40              |
| 25:RA:1812:A:O2'  | 27:RD:45:ASN:HB2   | 2.21                     | 0.40              |
| 27:RD:95:LEU:HD22 | 27:RD:117:VAL:HG11 | 2.02                     | 0.40              |
| 25:YA:384:U:H2'   | 25:YA:385:C:H6     | 1.87                     | 0.40              |
| 25:RA:1786:A:H1'  | 25:RA:1938:A:N6    | 2.37                     | 0.40              |
| 6:QF:7:ASN:OD1    | 6:QF:62:TRP:HD1    | 2.04                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 39:YT:130:ALA:HA | 39:YT:133:GLU:HG2 | 2.03                     | 0.40              |
| 45:RZ:5:LEU:HD21 | 45:RZ:44:PHE:HA   | 2.04                     | 0.40              |
| 7:QG:75:VAL:HG13 | 7:QG:145:ALA:HA   | 2.02                     | 0.40              |
| 22:QW:14:A:H8    | 22:QW:14:A:OP1    | 2.04                     | 0.40              |
| 35:RP:3:LEU:HD23 | 35:RP:3:LEU:HA    | 1.95                     | 0.40              |
| 1:XA:1479:C:H2'  | 1:XA:1480:G:C8    | 2.57                     | 0.40              |
| 25:RA:86:C:H4'   | 25:RA:104:U:H1'   | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | QB    | 234/256 (91%) | 186 (80%) | 29 (12%) | 19 (8%)  | 1           | 11  |
| 2   | XB    | 234/256 (91%) | 189 (81%) | 27 (12%) | 18 (8%)  | 1           | 12  |
| 3   | QC    | 204/239 (85%) | 162 (79%) | 26 (13%) | 16 (8%)  | 1           | 12  |
| 3   | XC    | 204/239 (85%) | 159 (78%) | 33 (16%) | 12 (6%)  | 2           | 19  |
| 4   | QD    | 206/209 (99%) | 169 (82%) | 26 (13%) | 11 (5%)  | 2           | 22  |
| 4   | XD    | 206/209 (99%) | 168 (82%) | 24 (12%) | 14 (7%)  | 1           | 16  |
| 5   | QE    | 152/162 (94%) | 136 (90%) | 12 (8%)  | 4 (3%)   | 7           | 42  |
| 5   | XE    | 152/162 (94%) | 137 (90%) | 10 (7%)  | 5 (3%)   | 5           | 37  |
| 6   | QF    | 99/101 (98%)  | 89 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 6   | XF    | 99/101 (98%)  | 95 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 7   | QG    | 153/156 (98%) | 136 (89%) | 13 (8%)  | 4 (3%)   | 7           | 42  |
| 7   | XG    | 153/156 (98%) | 134 (88%) | 15 (10%) | 4 (3%)   | 7           | 42  |
| 8   | QH    | 136/138 (99%) | 126 (93%) | 7 (5%)   | 3 (2%)   | 8           | 46  |
| 8   | XH    | 136/138 (99%) | 123 (90%) | 10 (7%)  | 3 (2%)   | 8           | 46  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 9   | QI    | 126/128 (98%) | 94 (75%)  | 24 (19%) | 8 (6%)   | 2           | 18  |
| 9   | XI    | 126/128 (98%) | 96 (76%)  | 23 (18%) | 7 (6%)   | 2           | 21  |
| 10  | QJ    | 97/105 (92%)  | 80 (82%)  | 13 (13%) | 4 (4%)   | 3           | 30  |
| 10  | XJ    | 97/105 (92%)  | 81 (84%)  | 11 (11%) | 5 (5%)   | 2           | 23  |
| 11  | QK    | 119/129 (92%) | 100 (84%) | 14 (12%) | 5 (4%)   | 3           | 29  |
| 11  | XK    | 119/129 (92%) | 105 (88%) | 10 (8%)  | 4 (3%)   | 5           | 36  |
| 12  | QL    | 123/132 (93%) | 99 (80%)  | 16 (13%) | 8 (6%)   | 1           | 17  |
| 12  | XL    | 123/132 (93%) | 97 (79%)  | 18 (15%) | 8 (6%)   | 1           | 17  |
| 13  | QM    | 116/126 (92%) | 88 (76%)  | 17 (15%) | 11 (10%) | 1           | 8   |
| 13  | XM    | 116/126 (92%) | 88 (76%)  | 17 (15%) | 11 (10%) | 1           | 8   |
| 14  | QN    | 58/61 (95%)   | 51 (88%)  | 4 (7%)   | 3 (5%)   | 2           | 23  |
| 14  | XN    | 58/61 (95%)   | 50 (86%)  | 5 (9%)   | 3 (5%)   | 2           | 23  |
| 15  | QO    | 86/89 (97%)   | 81 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 15  | XO    | 86/89 (97%)   | 79 (92%)  | 7 (8%)   | 0        | 100         | 100 |
| 16  | QP    | 82/88 (93%)   | 72 (88%)  | 10 (12%) | 0        | 100         | 100 |
| 16  | XP    | 82/88 (93%)   | 76 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 17  | QQ    | 98/105 (93%)  | 90 (92%)  | 7 (7%)   | 1 (1%)   | 19          | 63  |
| 17  | XQ    | 98/105 (93%)  | 89 (91%)  | 7 (7%)   | 2 (2%)   | 9           | 48  |
| 18  | QR    | 69/88 (78%)   | 61 (88%)  | 8 (12%)  | 0        | 100         | 100 |
| 18  | XR    | 69/88 (78%)   | 62 (90%)  | 6 (9%)   | 1 (1%)   | 14          | 55  |
| 19  | QS    | 80/93 (86%)   | 52 (65%)  | 18 (22%) | 10 (12%) | 0           | 4   |
| 19  | XS    | 80/93 (86%)   | 52 (65%)  | 18 (22%) | 10 (12%) | 0           | 4   |
| 20  | QT    | 97/106 (92%)  | 79 (81%)  | 15 (16%) | 3 (3%)   | 5           | 39  |
| 20  | XT    | 97/106 (92%)  | 80 (82%)  | 14 (14%) | 3 (3%)   | 5           | 39  |
| 21  | QU    | 23/27 (85%)   | 17 (74%)  | 5 (22%)  | 1 (4%)   | 3           | 29  |
| 21  | XU    | 23/27 (85%)   | 18 (78%)  | 3 (13%)  | 2 (9%)   | 1           | 10  |
| 24  | QY    | 89/117 (76%)  | 80 (90%)  | 9 (10%)  | 0        | 100         | 100 |
| 24  | XY    | 89/117 (76%)  | 84 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 27  | RD    | 270/276 (98%) | 224 (83%) | 38 (14%) | 8 (3%)   | 5           | 39  |
| 27  | YD    | 270/276 (98%) | 229 (85%) | 31 (12%) | 10 (4%)  | 4           | 33  |
| 28  | RE    | 203/206 (98%) | 141 (70%) | 36 (18%) | 26 (13%) | 0           | 4   |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 28  | YE    | 203/206 (98%) | 133 (66%) | 37 (18%) | 33 (16%) | 0           | 2  |
| 29  | RF    | 206/210 (98%) | 167 (81%) | 26 (13%) | 13 (6%)  | 2           | 18 |
| 29  | YF    | 206/210 (98%) | 168 (82%) | 22 (11%) | 16 (8%)  | 1           | 12 |
| 30  | RG    | 179/182 (98%) | 141 (79%) | 26 (14%) | 12 (7%)  | 1           | 16 |
| 30  | YG    | 179/182 (98%) | 147 (82%) | 21 (12%) | 11 (6%)  | 2           | 18 |
| 31  | RH    | 168/180 (93%) | 104 (62%) | 37 (22%) | 27 (16%) | 0           | 2  |
| 31  | YH    | 168/180 (93%) | 98 (58%)  | 42 (25%) | 28 (17%) | 0           | 2  |
| 32  | RI    | 144/148 (97%) | 110 (76%) | 28 (19%) | 6 (4%)   | 3           | 29 |
| 32  | YI    | 144/148 (97%) | 116 (81%) | 22 (15%) | 6 (4%)   | 3           | 29 |
| 33  | RN    | 136/140 (97%) | 116 (85%) | 13 (10%) | 7 (5%)   | 2           | 24 |
| 33  | YN    | 136/140 (97%) | 110 (81%) | 19 (14%) | 7 (5%)   | 2           | 24 |
| 34  | RO    | 120/122 (98%) | 111 (92%) | 8 (7%)   | 1 (1%)   | 24          | 67 |
| 34  | YO    | 120/122 (98%) | 109 (91%) | 10 (8%)  | 1 (1%)   | 24          | 67 |
| 35  | RP    | 148/150 (99%) | 99 (67%)  | 23 (16%) | 26 (18%) | 0           | 2  |
| 35  | YP    | 148/150 (99%) | 103 (70%) | 22 (15%) | 23 (16%) | 0           | 2  |
| 36  | RQ    | 138/141 (98%) | 110 (80%) | 17 (12%) | 11 (8%)  | 1           | 12 |
| 36  | YQ    | 137/141 (97%) | 111 (81%) | 15 (11%) | 11 (8%)  | 1           | 12 |
| 37  | RR    | 115/118 (98%) | 107 (93%) | 4 (4%)   | 4 (4%)   | 4           | 35 |
| 37  | YR    | 115/118 (98%) | 109 (95%) | 3 (3%)   | 3 (3%)   | 7           | 42 |
| 38  | RS    | 109/112 (97%) | 84 (77%)  | 17 (16%) | 8 (7%)   | 1           | 14 |
| 38  | YS    | 109/112 (97%) | 85 (78%)  | 13 (12%) | 11 (10%) | 1           | 7  |
| 39  | RT    | 135/146 (92%) | 108 (80%) | 25 (18%) | 2 (2%)   | 13          | 54 |
| 39  | YT    | 135/146 (92%) | 113 (84%) | 17 (13%) | 5 (4%)   | 4           | 33 |
| 40  | RU    | 115/118 (98%) | 107 (93%) | 6 (5%)   | 2 (2%)   | 11          | 51 |
| 40  | YU    | 115/118 (98%) | 103 (90%) | 9 (8%)   | 3 (3%)   | 7           | 42 |
| 41  | RV    | 99/101 (98%)  | 71 (72%)  | 13 (13%) | 15 (15%) | 0           | 2  |
| 41  | YV    | 99/101 (98%)  | 70 (71%)  | 15 (15%) | 14 (14%) | 0           | 3  |
| 42  | RW    | 111/113 (98%) | 107 (96%) | 1 (1%)   | 3 (3%)   | 6           | 41 |
| 42  | YW    | 111/113 (98%) | 104 (94%) | 3 (3%)   | 4 (4%)   | 4           | 34 |
| 43  | RX    | 90/96 (94%)   | 77 (86%)  | 11 (12%) | 2 (2%)   | 8           | 46 |
| 43  | YX    | 90/96 (94%)   | 77 (86%)  | 11 (12%) | 2 (2%)   | 8           | 46 |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 44  | RY    | 100/110 (91%)     | 57 (57%)   | 28 (28%)   | 15 (15%) | 0           | 2   |
| 44  | YY    | 100/110 (91%)     | 58 (58%)   | 26 (26%)   | 16 (16%) | 0           | 2   |
| 45  | RZ    | 174/206 (84%)     | 119 (68%)  | 33 (19%)   | 22 (13%) | 0           | 4   |
| 45  | YZ    | 181/206 (88%)     | 122 (67%)  | 42 (23%)   | 17 (9%)  | 1           | 8   |
| 46  | R0    | 81/85 (95%)       | 73 (90%)   | 5 (6%)     | 3 (4%)   | 4           | 33  |
| 46  | Y0    | 81/85 (95%)       | 67 (83%)   | 11 (14%)   | 3 (4%)   | 4           | 33  |
| 47  | R1    | 95/98 (97%)       | 71 (75%)   | 12 (13%)   | 12 (13%) | 0           | 4   |
| 47  | Y1    | 95/98 (97%)       | 76 (80%)   | 13 (14%)   | 6 (6%)   | 2           | 18  |
| 48  | R2    | 67/72 (93%)       | 54 (81%)   | 8 (12%)    | 5 (8%)   | 1           | 13  |
| 48  | Y2    | 67/72 (93%)       | 56 (84%)   | 5 (8%)     | 6 (9%)   | 1           | 9   |
| 49  | R3    | 57/60 (95%)       | 51 (90%)   | 6 (10%)    | 0        | 100         | 100 |
| 49  | Y3    | 57/60 (95%)       | 51 (90%)   | 6 (10%)    | 0        | 100         | 100 |
| 50  | R4    | 68/71 (96%)       | 43 (63%)   | 12 (18%)   | 13 (19%) | 0           | 1   |
| 50  | Y4    | 68/71 (96%)       | 37 (54%)   | 15 (22%)   | 16 (24%) | 0           | 1   |
| 51  | R5    | 57/60 (95%)       | 46 (81%)   | 9 (16%)    | 2 (4%)   | 4           | 35  |
| 51  | Y5    | 55/60 (92%)       | 48 (87%)   | 3 (6%)     | 4 (7%)   | 1           | 14  |
| 52  | R6    | 46/54 (85%)       | 22 (48%)   | 15 (33%)   | 9 (20%)  | 0           | 1   |
| 52  | Y6    | 46/54 (85%)       | 16 (35%)   | 17 (37%)   | 13 (28%) | 0           | 0   |
| 53  | R7    | 47/49 (96%)       | 47 (100%)  | 0          | 0        | 100         | 100 |
| 53  | Y7    | 47/49 (96%)       | 44 (94%)   | 3 (6%)     | 0        | 100         | 100 |
| 54  | R8    | 62/65 (95%)       | 48 (77%)   | 7 (11%)    | 7 (11%)  | 0           | 6   |
| 54  | Y8    | 62/65 (95%)       | 48 (77%)   | 7 (11%)    | 7 (11%)  | 0           | 6   |
| 55  | R9    | 35/37 (95%)       | 34 (97%)   | 0          | 1 (3%)   | 6           | 40  |
| 55  | Y9    | 34/37 (92%)       | 33 (97%)   | 1 (3%)     | 0        | 100         | 100 |
| All | All   | 11647/12362 (94%) | 9400 (81%) | 1486 (13%) | 761 (6%) | 1           | 17  |

All (761) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 29  | ALA  |
| 2   | QB    | 165 | VAL  |
| 2   | QB    | 195 | ASP  |
| 2   | QB    | 238 | LEU  |
| 3   | QC    | 64  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | QC    | 77  | ILE  |
| 4   | QD    | 13  | ARG  |
| 4   | QD    | 14  | ARG  |
| 4   | QD    | 24  | GLU  |
| 4   | QD    | 34  | GLU  |
| 4   | QD    | 150 | GLU  |
| 5   | QE    | 115 | VAL  |
| 7   | QG    | 80  | VAL  |
| 9   | QI    | 34  | ASN  |
| 9   | QI    | 35  | GLU  |
| 10  | QJ    | 75  | ILE  |
| 12  | QL    | 47  | LYS  |
| 12  | QL    | 79  | GLU  |
| 13  | QM    | 12  | ASN  |
| 13  | QM    | 14  | ARG  |
| 13  | QM    | 47  | ASP  |
| 13  | QM    | 83  | ASP  |
| 17  | QQ    | 69  | LYS  |
| 19  | QS    | 37  | ARG  |
| 19  | QS    | 67  | VAL  |
| 19  | QS    | 70  | LYS  |
| 19  | QS    | 72  | GLY  |
| 27  | RD    | 28  | GLU  |
| 28  | RE    | 53  | PRO  |
| 28  | RE    | 63  | LEU  |
| 28  | RE    | 64  | LYS  |
| 28  | RE    | 68  | ALA  |
| 28  | RE    | 71  | GLY  |
| 29  | RF    | 2   | LYS  |
| 29  | RF    | 25  | PRO  |
| 29  | RF    | 132 | VAL  |
| 30  | RG    | 97  | ASP  |
| 31  | RH    | 9   | ILE  |
| 31  | RH    | 10  | PRO  |
| 31  | RH    | 12  | PRO  |
| 31  | RH    | 15  | VAL  |
| 31  | RH    | 49  | VAL  |
| 31  | RH    | 80  | SER  |
| 31  | RH    | 152 | ARG  |
| 31  | RH    | 153 | LYS  |
| 31  | RH    | 164 | TYR  |
| 31  | RH    | 168 | PRO  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 32         | RI           | 144        | VAL         |
| 33         | RN           | 131        | GLN         |
| 34         | RO           | 48         | PRO         |
| 35         | RP           | 6          | LEU         |
| 35         | RP           | 10         | PRO         |
| 35         | RP           | 15         | ARG         |
| 35         | RP           | 27         | HIS         |
| 35         | RP           | 29         | LYS         |
| 35         | RP           | 42         | SER         |
| 35         | RP           | 56         | SER         |
| 35         | RP           | 57         | THR         |
| 35         | RP           | 62         | LEU         |
| 35         | RP           | 63         | PRO         |
| 35         | RP           | 98         | GLU         |
| 36         | RQ           | 78         | PRO         |
| 36         | RQ           | 90         | VAL         |
| 36         | RQ           | 133        | ARG         |
| 38         | RS           | 89         | ARG         |
| 41         | RV           | 47         | VAL         |
| 41         | RV           | 49         | THR         |
| 44         | RY           | 77         | PRO         |
| 44         | RY           | 78         | ALA         |
| 44         | RY           | 85         | VAL         |
| 44         | RY           | 89         | PHE         |
| 45         | RZ           | 53         | ILE         |
| 45         | RZ           | 157        | LEU         |
| 46         | R0           | 47         | PRO         |
| 47         | R1           | 30         | VAL         |
| 47         | R1           | 45         | ASN         |
| 48         | R2           | 47         | ASN         |
| 50         | R4           | 39         | CYS         |
| 50         | R4           | 40         | HIS         |
| 51         | R5           | 4          | HIS         |
| 52         | R6           | 19         | ARG         |
| 52         | R6           | 31         | PRO         |
| 54         | R8           | 32         | LEU         |
| 54         | R8           | 34         | TRP         |
| 55         | R9           | 2          | LYS         |
| 2          | XB           | 15         | VAL         |
| 2          | XB           | 29         | ALA         |
| 2          | XB           | 165        | VAL         |
| 2          | XB           | 190        | THR         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | XB    | 238 | LEU  |
| 3   | XC    | 12  | LEU  |
| 3   | XC    | 64  | VAL  |
| 4   | XD    | 14  | ARG  |
| 4   | XD    | 24  | GLU  |
| 4   | XD    | 26  | CYS  |
| 4   | XD    | 110 | PHE  |
| 5   | XE    | 115 | VAL  |
| 7   | XG    | 80  | VAL  |
| 9   | XI    | 118 | LYS  |
| 10  | XJ    | 54  | PHE  |
| 10  | XJ    | 57  | LYS  |
| 10  | XJ    | 75  | ILE  |
| 12  | XL    | 127 | GLU  |
| 13  | XM    | 3   | ARG  |
| 13  | XM    | 14  | ARG  |
| 13  | XM    | 47  | ASP  |
| 13  | XM    | 83  | ASP  |
| 14  | XN    | 15  | LYS  |
| 18  | XR    | 20  | ALA  |
| 19  | XS    | 37  | ARG  |
| 19  | XS    | 38  | SER  |
| 19  | XS    | 70  | LYS  |
| 27  | YD    | 26  | LYS  |
| 27  | YD    | 28  | GLU  |
| 28  | YE    | 54  | GLN  |
| 28  | YE    | 61  | ARG  |
| 28  | YE    | 64  | LYS  |
| 28  | YE    | 78  | LEU  |
| 29  | YF    | 25  | PRO  |
| 29  | YF    | 67  | GLN  |
| 29  | YF    | 123 | LEU  |
| 29  | YF    | 124 | LEU  |
| 31  | YH    | 9   | ILE  |
| 31  | YH    | 10  | PRO  |
| 31  | YH    | 15  | VAL  |
| 31  | YH    | 49  | VAL  |
| 31  | YH    | 84  | SER  |
| 31  | YH    | 109 | PHE  |
| 31  | YH    | 152 | ARG  |
| 31  | YH    | 153 | LYS  |
| 31  | YH    | 168 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | YI    | 141 | LYS  |
| 33  | YN    | 17  | ASP  |
| 33  | YN    | 18  | ALA  |
| 34  | YO    | 48  | PRO  |
| 35  | YP    | 6   | LEU  |
| 35  | YP    | 10  | PRO  |
| 35  | YP    | 15  | ARG  |
| 35  | YP    | 16  | ARG  |
| 35  | YP    | 27  | HIS  |
| 35  | YP    | 45  | LEU  |
| 35  | YP    | 56  | SER  |
| 35  | YP    | 62  | LEU  |
| 35  | YP    | 63  | PRO  |
| 36  | YQ    | 18  | LYS  |
| 36  | YQ    | 59  | ARG  |
| 36  | YQ    | 78  | PRO  |
| 36  | YQ    | 133 | ARG  |
| 38  | YS    | 89  | ARG  |
| 38  | YS    | 107 | GLU  |
| 41  | YV    | 85  | LYS  |
| 44  | YY    | 77  | PRO  |
| 44  | YY    | 78  | ALA  |
| 44  | YY    | 80  | GLY  |
| 44  | YY    | 89  | PHE  |
| 45  | YZ    | 53  | ILE  |
| 45  | YZ    | 111 | VAL  |
| 45  | YZ    | 141 | VAL  |
| 45  | YZ    | 154 | ASP  |
| 46  | Y0    | 47  | PRO  |
| 47  | Y1    | 30  | VAL  |
| 47  | Y1    | 93  | GLU  |
| 48  | Y2    | 43  | GLN  |
| 48  | Y2    | 47  | ASN  |
| 50  | Y4    | 6   | HIS  |
| 50  | Y4    | 40  | HIS  |
| 51  | Y5    | 4   | HIS  |
| 52  | Y6    | 28  | ARG  |
| 52  | Y6    | 31  | PRO  |
| 54  | Y8    | 30  | ARG  |
| 54  | Y8    | 33  | ASN  |
| 54  | Y8    | 51  | ALA  |
| 54  | Y8    | 61  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 16  | HIS  |
| 2   | QB    | 20  | GLU  |
| 2   | QB    | 39  | ILE  |
| 2   | QB    | 194 | PRO  |
| 3   | QC    | 12  | LEU  |
| 3   | QC    | 78  | GLY  |
| 3   | QC    | 85  | ARG  |
| 3   | QC    | 160 | ALA  |
| 3   | QC    | 162 | GLN  |
| 7   | QG    | 17  | VAL  |
| 8   | QH    | 99  | GLU  |
| 9   | QI    | 119 | ALA  |
| 9   | QI    | 124 | GLN  |
| 10  | QJ    | 54  | PHE  |
| 11  | QK    | 10  | VAL  |
| 11  | QK    | 15  | ALA  |
| 12  | QL    | 45  | PRO  |
| 12  | QL    | 127 | GLU  |
| 13  | QM    | 3   | ARG  |
| 13  | QM    | 48  | LEU  |
| 13  | QM    | 63  | THR  |
| 13  | QM    | 100 | GLY  |
| 13  | QM    | 116 | THR  |
| 14  | QN    | 14  | PRO  |
| 14  | QN    | 15  | LYS  |
| 19  | QS    | 38  | SER  |
| 19  | QS    | 41  | VAL  |
| 19  | QS    | 80  | TYR  |
| 27  | RD    | 25  | THR  |
| 27  | RD    | 33  | LEU  |
| 27  | RD    | 159 | ALA  |
| 27  | RD    | 196 | VAL  |
| 27  | RD    | 239 | ARG  |
| 28  | RE    | 48  | GLN  |
| 28  | RE    | 50  | GLY  |
| 28  | RE    | 60  | ASN  |
| 28  | RE    | 66  | HIS  |
| 28  | RE    | 72  | VAL  |
| 29  | RF    | 3   | GLU  |
| 29  | RF    | 28  | ILE  |
| 29  | RF    | 67  | GLN  |
| 29  | RF    | 123 | LEU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 29         | RF           | 124        | LEU         |
| 31         | RH           | 11         | VAL         |
| 31         | RH           | 45         | VAL         |
| 31         | RH           | 55         | PRO         |
| 31         | RH           | 109        | PHE         |
| 31         | RH           | 151        | ILE         |
| 32         | RI           | 77         | LEU         |
| 33         | RN           | 18         | ALA         |
| 35         | RP           | 21         | ARG         |
| 35         | RP           | 24         | GLY         |
| 35         | RP           | 147        | LEU         |
| 36         | RQ           | 80         | GLU         |
| 36         | RQ           | 134        | ARG         |
| 36         | RQ           | 135        | ASP         |
| 36         | RQ           | 136        | ALA         |
| 38         | RS           | 4          | LEU         |
| 38         | RS           | 44         | LYS         |
| 38         | RS           | 88         | ASP         |
| 38         | RS           | 94         | TYR         |
| 39         | RT           | 86         | ILE         |
| 40         | RU           | 92         | ARG         |
| 41         | RV           | 72         | VAL         |
| 41         | RV           | 80         | GLN         |
| 41         | RV           | 84         | LYS         |
| 41         | RV           | 85         | LYS         |
| 41         | RV           | 87         | HIS         |
| 41         | RV           | 98         | GLU         |
| 42         | RW           | 63         | ASP         |
| 43         | RX           | 67         | GLY         |
| 44         | RY           | 61         | ILE         |
| 44         | RY           | 63         | LYS         |
| 44         | RY           | 80         | GLY         |
| 44         | RY           | 99         | CYS         |
| 45         | RZ           | 51         | ALA         |
| 45         | RZ           | 59         | LEU         |
| 45         | RZ           | 115        | GLY         |
| 45         | RZ           | 119        | GLU         |
| 45         | RZ           | 142        | SER         |
| 45         | RZ           | 151        | HIS         |
| 45         | RZ           | 165        | VAL         |
| 47         | R1           | 27         | GLU         |
| 47         | R1           | 82         | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 47         | R1           | 92         | LYS         |
| 47         | R1           | 93         | GLU         |
| 48         | R2           | 48         | HIS         |
| 50         | R4           | 5          | ILE         |
| 50         | R4           | 48         | ARG         |
| 50         | R4           | 51         | ASP         |
| 52         | R6           | 14         | THR         |
| 54         | R8           | 30         | ARG         |
| 54         | R8           | 55         | ALA         |
| 54         | R8           | 61         | LEU         |
| 2          | XB           | 191        | ASP         |
| 3          | XC           | 84         | ILE         |
| 3          | XC           | 160        | ALA         |
| 3          | XC           | 162        | GLN         |
| 4          | XD           | 20         | TYR         |
| 4          | XD           | 23         | GLY         |
| 4          | XD           | 27         | TYR         |
| 4          | XD           | 29         | PRO         |
| 7          | XG           | 21         | VAL         |
| 8          | XH           | 99         | GLU         |
| 9          | XI           | 124        | GLN         |
| 12         | XL           | 19         | ARG         |
| 12         | XL           | 92         | ASP         |
| 12         | XL           | 128        | ALA         |
| 13         | XM           | 100        | GLY         |
| 14         | XN           | 14         | PRO         |
| 14         | XN           | 16         | PHE         |
| 17         | XQ           | 69         | LYS         |
| 19         | XS           | 25         | LYS         |
| 19         | XS           | 80         | TYR         |
| 21         | XU           | 25         | LYS         |
| 27         | YD           | 33         | LEU         |
| 27         | YD           | 196        | VAL         |
| 27         | YD           | 238        | GLY         |
| 27         | YD           | 267        | SER         |
| 28         | YE           | 9          | VAL         |
| 28         | YE           | 25         | VAL         |
| 28         | YE           | 59         | VAL         |
| 28         | YE           | 69         | LYS         |
| 28         | YE           | 71         | GLY         |
| 28         | YE           | 76         | ARG         |
| 28         | YE           | 77         | ILE         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 28         | YE           | 118        | LYS         |
| 28         | YE           | 132        | HIS         |
| 29         | YF           | 3          | GLU         |
| 29         | YF           | 84         | VAL         |
| 30         | YG           | 14         | GLU         |
| 30         | YG           | 96         | ARG         |
| 30         | YG           | 97         | ASP         |
| 31         | YH           | 11         | VAL         |
| 31         | YH           | 55         | PRO         |
| 31         | YH           | 80         | SER         |
| 32         | YI           | 102        | SER         |
| 32         | YI           | 145        | VAL         |
| 33         | YN           | 126        | PRO         |
| 35         | YP           | 29         | LYS         |
| 35         | YP           | 57         | THR         |
| 36         | YQ           | 81         | VAL         |
| 36         | YQ           | 86         | GLY         |
| 36         | YQ           | 90         | VAL         |
| 36         | YQ           | 134        | ARG         |
| 36         | YQ           | 135        | ASP         |
| 36         | YQ           | 136        | ALA         |
| 38         | YS           | 19         | LYS         |
| 38         | YS           | 88         | ASP         |
| 38         | YS           | 94         | TYR         |
| 38         | YS           | 96         | GLY         |
| 39         | YT           | 84         | GLN         |
| 39         | YT           | 107        | ASP         |
| 40         | YU           | 90         | VAL         |
| 40         | YU           | 101        | ARG         |
| 41         | YV           | 44         | LYS         |
| 41         | YV           | 45         | THR         |
| 41         | YV           | 50         | PRO         |
| 41         | YV           | 62         | LEU         |
| 41         | YV           | 72         | VAL         |
| 41         | YV           | 80         | GLN         |
| 42         | YW           | 63         | ASP         |
| 42         | YW           | 93         | ALA         |
| 44         | YY           | 61         | ILE         |
| 44         | YY           | 63         | LYS         |
| 44         | YY           | 99         | CYS         |
| 45         | YZ           | 60         | GLU         |
| 45         | YZ           | 142        | SER         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 45         | YZ           | 146        | ILE         |
| 48         | Y2           | 70         | GLN         |
| 50         | Y4           | 11         | PRO         |
| 50         | Y4           | 22         | ILE         |
| 50         | Y4           | 23         | GLU         |
| 50         | Y4           | 24         | THR         |
| 50         | Y4           | 39         | CYS         |
| 50         | Y4           | 42         | PHE         |
| 50         | Y4           | 48         | ARG         |
| 50         | Y4           | 51         | ASP         |
| 51         | Y5           | 55         | ARG         |
| 52         | Y6           | 19         | ARG         |
| 52         | Y6           | 27         | LYS         |
| 52         | Y6           | 29         | ASN         |
| 54         | Y8           | 7          | HIS         |
| 54         | Y8           | 55         | ALA         |
| 2          | QB           | 8          | LYS         |
| 2          | QB           | 28         | PHE         |
| 2          | QB           | 88         | ALA         |
| 2          | QB           | 133        | LYS         |
| 2          | QB           | 191        | ASP         |
| 2          | QB           | 239        | VAL         |
| 3          | QC           | 15         | THR         |
| 4          | QD           | 22         | LYS         |
| 4          | QD           | 32         | ALA         |
| 5          | QE           | 19         | MET         |
| 8          | QH           | 2          | LEU         |
| 9          | QI           | 21         | PRO         |
| 9          | QI           | 29         | ASN         |
| 10         | QJ           | 59         | SER         |
| 12         | QL           | 25         | PRO         |
| 12         | QL           | 128        | ALA         |
| 14         | QN           | 16         | PHE         |
| 20         | QT           | 97         | ALA         |
| 20         | QT           | 103        | GLY         |
| 21         | QU           | 25         | LYS         |
| 28         | RE           | 2          | LYS         |
| 28         | RE           | 25         | VAL         |
| 28         | RE           | 32         | PRO         |
| 28         | RE           | 80         | GLU         |
| 28         | RE           | 92         | THR         |
| 28         | RE           | 204        | ALA         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | RF    | 21  | ALA  |
| 30  | RG    | 82  | LEU  |
| 30  | RG    | 96  | ARG  |
| 30  | RG    | 116 | ASP  |
| 31  | RH    | 27  | LYS  |
| 31  | RH    | 47  | GLU  |
| 31  | RH    | 85  | LYS  |
| 31  | RH    | 160 | LYS  |
| 32  | RI    | 85  | GLU  |
| 32  | RI    | 102 | SER  |
| 32  | RI    | 117 | GLU  |
| 33  | RN    | 17  | ASP  |
| 35  | RP    | 103 | ALA  |
| 35  | RP    | 141 | ALA  |
| 37  | RR    | 107 | ASP  |
| 39  | RT    | 107 | ASP  |
| 40  | RU    | 98  | LEU  |
| 41  | RV    | 44  | LYS  |
| 41  | RV    | 62  | LEU  |
| 41  | RV    | 71  | LEU  |
| 44  | RY    | 3   | VAL  |
| 44  | RY    | 17  | SER  |
| 44  | RY    | 19  | LYS  |
| 44  | RY    | 53  | PRO  |
| 45  | RZ    | 13  | GLU  |
| 45  | RZ    | 163 | LEU  |
| 46  | R0    | 83  | PRO  |
| 47  | R1    | 55  | GLY  |
| 47  | R1    | 96  | LYS  |
| 48  | R2    | 43  | GLN  |
| 50  | R4    | 24  | THR  |
| 50  | R4    | 42  | PHE  |
| 50  | R4    | 52  | THR  |
| 52  | R6    | 49  | HIS  |
| 54  | R8    | 51  | ALA  |
| 2   | XB    | 16  | HIS  |
| 2   | XB    | 20  | GLU  |
| 2   | XB    | 26  | PRO  |
| 2   | XB    | 39  | ILE  |
| 2   | XB    | 133 | LYS  |
| 3   | XC    | 15  | THR  |
| 3   | XC    | 51  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | XC    | 53  | ALA  |
| 3   | XC    | 77  | ILE  |
| 4   | XD    | 34  | GLU  |
| 4   | XD    | 150 | GLU  |
| 5   | XE    | 3   | GLU  |
| 5   | XE    | 7   | GLU  |
| 5   | XE    | 39  | GLY  |
| 8   | XH    | 2   | LEU  |
| 10  | XJ    | 91  | PRO  |
| 11  | XK    | 15  | ALA  |
| 13  | XM    | 82  | MET  |
| 13  | XM    | 116 | THR  |
| 17  | XQ    | 74  | LEU  |
| 19  | XS    | 67  | VAL  |
| 20  | XT    | 10  | LEU  |
| 20  | XT    | 103 | GLY  |
| 21  | XU    | 3   | LYS  |
| 27  | YD    | 25  | THR  |
| 27  | YD    | 159 | ALA  |
| 28  | YE    | 2   | LYS  |
| 28  | YE    | 48  | GLN  |
| 28  | YE    | 51  | PHE  |
| 28  | YE    | 131 | ALA  |
| 28  | YE    | 187 | ALA  |
| 28  | YE    | 204 | ALA  |
| 29  | YF    | 9   | ILE  |
| 29  | YF    | 17  | ARG  |
| 29  | YF    | 62  | ARG  |
| 29  | YF    | 128 | ALA  |
| 29  | YF    | 133 | ASN  |
| 30  | YG    | 5   | VAL  |
| 31  | YH    | 12  | PRO  |
| 31  | YH    | 21  | PRO  |
| 31  | YH    | 47  | GLU  |
| 31  | YH    | 90  | LYS  |
| 31  | YH    | 130 | ARG  |
| 32  | YI    | 77  | LEU  |
| 33  | YN    | 127 | ASP  |
| 33  | YN    | 131 | GLN  |
| 35  | YP    | 5   | ASP  |
| 35  | YP    | 47  | ASP  |
| 35  | YP    | 107 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | YP    | 141 | ALA  |
| 38  | YS    | 12  | PHE  |
| 38  | YS    | 44  | LYS  |
| 39  | YT    | 86  | ILE  |
| 40  | YU    | 92  | ARG  |
| 42  | YW    | 110 | LYS  |
| 44  | YY    | 53  | PRO  |
| 44  | YY    | 58  | GLY  |
| 45  | YZ    | 6   | LYS  |
| 45  | YZ    | 13  | GLU  |
| 45  | YZ    | 73  | GLN  |
| 45  | YZ    | 136 | PHE  |
| 45  | YZ    | 150 | LEU  |
| 45  | YZ    | 173 | ALA  |
| 46  | Y0    | 83  | PRO  |
| 47  | Y1    | 79  | GLY  |
| 47  | Y1    | 96  | LYS  |
| 48  | Y2    | 48  | HIS  |
| 50  | Y4    | 34  | GLU  |
| 50  | Y4    | 52  | THR  |
| 52  | Y6    | 11  | LEU  |
| 52  | Y6    | 49  | HIS  |
| 2   | QB    | 131 | PRO  |
| 2   | QB    | 234 | PRO  |
| 3   | QC    | 13  | GLY  |
| 3   | QC    | 16  | ARG  |
| 3   | QC    | 206 | GLU  |
| 4   | QD    | 26  | CYS  |
| 4   | QD    | 149 | ALA  |
| 5   | QE    | 7   | GLU  |
| 7   | QG    | 7   | ALA  |
| 8   | QH    | 100 | ILE  |
| 9   | QI    | 19  | LEU  |
| 11  | QK    | 16  | SER  |
| 12  | QL    | 19  | ARG  |
| 13  | QM    | 82  | MET  |
| 19  | QS    | 43  | GLU  |
| 19  | QS    | 65  | ASN  |
| 27  | RD    | 3   | VAL  |
| 28  | RE    | 9   | VAL  |
| 28  | RE    | 33  | VAL  |
| 28  | RE    | 45  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | RE    | 86  | PRO  |
| 28  | RE    | 90  | THR  |
| 28  | RE    | 129 | HIS  |
| 28  | RE    | 200 | GLU  |
| 29  | RF    | 17  | ARG  |
| 29  | RF    | 133 | ASN  |
| 30  | RG    | 5   | VAL  |
| 30  | RG    | 14  | GLU  |
| 30  | RG    | 36  | LYS  |
| 30  | RG    | 86  | MET  |
| 31  | RH    | 7   | LEU  |
| 31  | RH    | 34  | GLU  |
| 31  | RH    | 39  | PRO  |
| 31  | RH    | 111 | HIS  |
| 31  | RH    | 169 | VAL  |
| 32  | RI    | 132 | PRO  |
| 33  | RN    | 126 | PRO  |
| 33  | RN    | 127 | ASP  |
| 35  | RP    | 61  | ARG  |
| 35  | RP    | 111 | ARG  |
| 36  | RQ    | 59  | ARG  |
| 36  | RQ    | 104 | PHE  |
| 37  | RR    | 82  | GLU  |
| 38  | RS    | 106 | ARG  |
| 44  | RY    | 57  | GLN  |
| 44  | RY    | 58  | GLY  |
| 44  | RY    | 73  | ARG  |
| 45  | RZ    | 6   | LYS  |
| 45  | RZ    | 118 | GLN  |
| 45  | RZ    | 136 | PHE  |
| 46  | R0    | 49  | LYS  |
| 48  | R2    | 16  | LEU  |
| 50  | R4    | 46  | GLN  |
| 50  | R4    | 50  | VAL  |
| 51  | R5    | 49  | CYS  |
| 52  | R6    | 22  | ALA  |
| 54  | R8    | 7   | HIS  |
| 2   | XB    | 95  | GLN  |
| 2   | XB    | 122 | PHE  |
| 2   | XB    | 226 | ARG  |
| 3   | XC    | 79  | ARG  |
| 4   | XD    | 16  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | XD    | 25  | ARG  |
| 4   | XD    | 149 | ALA  |
| 7   | XG    | 7   | ALA  |
| 8   | XH    | 100 | ILE  |
| 9   | XI    | 19  | LEU  |
| 11  | XK    | 12  | ARG  |
| 12  | XL    | 47  | LYS  |
| 13  | XM    | 45  | VAL  |
| 13  | XM    | 63  | THR  |
| 27  | YD    | 46  | GLN  |
| 27  | YD    | 239 | ARG  |
| 28  | YE    | 32  | PRO  |
| 28  | YE    | 66  | HIS  |
| 28  | YE    | 90  | THR  |
| 29  | YF    | 21  | ALA  |
| 29  | YF    | 89  | VAL  |
| 30  | YG    | 36  | LYS  |
| 30  | YG    | 82  | LEU  |
| 30  | YG    | 109 | VAL  |
| 30  | YG    | 116 | ASP  |
| 30  | YG    | 117 | PHE  |
| 31  | YH    | 4   | ILE  |
| 31  | YH    | 30  | LYS  |
| 31  | YH    | 39  | PRO  |
| 31  | YH    | 85  | LYS  |
| 31  | YH    | 160 | LYS  |
| 32  | YI    | 132 | PRO  |
| 35  | YP    | 12  | ALA  |
| 35  | YP    | 21  | ARG  |
| 35  | YP    | 111 | ARG  |
| 35  | YP    | 147 | LEU  |
| 36  | YQ    | 104 | PHE  |
| 37  | YR    | 82  | GLU  |
| 37  | YR    | 107 | ASP  |
| 38  | YS    | 4   | LEU  |
| 38  | YS    | 57  | LYS  |
| 39  | YT    | 105 | LEU  |
| 41  | YV    | 79  | VAL  |
| 41  | YV    | 98  | GLU  |
| 42  | YW    | 65  | LEU  |
| 44  | YY    | 50  | ARG  |
| 44  | YY    | 73  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | YY    | 96  | ILE  |
| 45  | YZ    | 157 | LEU  |
| 46  | Y0    | 49  | LYS  |
| 47  | Y1    | 92  | LYS  |
| 50  | Y4    | 46  | GLN  |
| 51  | Y5    | 7   | PRO  |
| 51  | Y5    | 49  | CYS  |
| 52  | Y6    | 25  | LYS  |
| 52  | Y6    | 44  | ARG  |
| 2   | QB    | 150 | SER  |
| 3   | QC    | 3   | ASN  |
| 3   | QC    | 45  | LYS  |
| 3   | QC    | 84  | ILE  |
| 3   | QC    | 98  | ASN  |
| 4   | QD    | 5   | ILE  |
| 4   | QD    | 39  | PRO  |
| 7   | QG    | 19  | GLY  |
| 9   | QI    | 107 | ARG  |
| 10  | QJ    | 37  | PRO  |
| 11  | QK    | 11  | LYS  |
| 12  | QL    | 92  | ASP  |
| 13  | QM    | 45  | VAL  |
| 27  | RD    | 191 | ALA  |
| 28  | RE    | 54  | GLN  |
| 28  | RE    | 82  | ARG  |
| 29  | RF    | 9   | ILE  |
| 29  | RF    | 66  | PRO  |
| 30  | RG    | 117 | PHE  |
| 31  | RH    | 46  | GLU  |
| 31  | RH    | 52  | VAL  |
| 33  | RN    | 125 | GLY  |
| 33  | RN    | 129 | PRO  |
| 35  | RP    | 16  | ARG  |
| 35  | RP    | 47  | ASP  |
| 36  | RQ    | 81  | VAL  |
| 37  | RR    | 103 | ARG  |
| 37  | RR    | 106 | GLY  |
| 38  | RS    | 19  | LYS  |
| 38  | RS    | 87  | PHE  |
| 41  | RV    | 99  | ILE  |
| 42  | RW    | 93  | ALA  |
| 43  | RX    | 51  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | RZ    | 73  | GLN  |
| 45  | RZ    | 146 | ILE  |
| 45  | RZ    | 173 | ALA  |
| 47  | R1    | 81  | LYS  |
| 50  | R4    | 11  | PRO  |
| 50  | R4    | 23  | GLU  |
| 52  | R6    | 20  | ASN  |
| 52  | R6    | 27  | LYS  |
| 2   | XB    | 131 | PRO  |
| 2   | XB    | 231 | GLU  |
| 2   | XB    | 234 | PRO  |
| 2   | XB    | 239 | VAL  |
| 3   | XC    | 16  | ARG  |
| 3   | XC    | 99  | VAL  |
| 4   | XD    | 5   | ILE  |
| 12  | XL    | 17  | LYS  |
| 12  | XL    | 79  | GLU  |
| 19  | XS    | 41  | VAL  |
| 28  | YE    | 44  | TYR  |
| 28  | YE    | 45  | THR  |
| 28  | YE    | 47  | VAL  |
| 28  | YE    | 62  | PRO  |
| 28  | YE    | 73  | GLU  |
| 28  | YE    | 82  | ARG  |
| 29  | YF    | 27  | GLU  |
| 29  | YF    | 28  | ILE  |
| 30  | YG    | 86  | MET  |
| 31  | YH    | 7   | LEU  |
| 31  | YH    | 52  | VAL  |
| 31  | YH    | 87  | LEU  |
| 31  | YH    | 111 | HIS  |
| 31  | YH    | 169 | VAL  |
| 33  | YN    | 8   | GLN  |
| 33  | YN    | 129 | PRO  |
| 35  | YP    | 19  | VAL  |
| 35  | YP    | 106 | LEU  |
| 38  | YS    | 87  | PHE  |
| 39  | YT    | 97  | ALA  |
| 41  | YV    | 29  | PRO  |
| 41  | YV    | 36  | PRO  |
| 41  | YV    | 99  | ILE  |
| 43  | YX    | 51  | VAL  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 44         | YY           | 16         | ALA         |
| 44         | YY           | 85         | VAL         |
| 45         | YZ           | 156        | LYS         |
| 48         | Y2           | 16         | LEU         |
| 48         | Y2           | 44         | LEU         |
| 50         | Y4           | 50         | VAL         |
| 50         | Y4           | 57         | GLU         |
| 20         | QT           | 98         | PRO         |
| 36         | RQ           | 63         | LYS         |
| 41         | RV           | 37         | VAL         |
| 42         | RW           | 65         | LEU         |
| 45         | RZ           | 67         | LEU         |
| 47         | R1           | 31         | GLY         |
| 47         | R1           | 86         | SER         |
| 52         | R6           | 11         | LEU         |
| 9          | XI           | 30         | GLY         |
| 11         | XK           | 10         | VAL         |
| 11         | XK           | 105        | VAL         |
| 12         | XL           | 65         | GLU         |
| 19         | XS           | 9          | VAL         |
| 19         | XS           | 72         | GLY         |
| 28         | YE           | 134        | ILE         |
| 30         | YG           | 146        | TYR         |
| 31         | YH           | 151        | ILE         |
| 44         | YY           | 41         | GLY         |
| 45         | YZ           | 59         | LEU         |
| 45         | YZ           | 165        | VAL         |
| 47         | Y1           | 27         | GLU         |
| 50         | Y4           | 7          | PRO         |
| 52         | Y6           | 12         | GLU         |
| 52         | Y6           | 22         | ALA         |
| 52         | Y6           | 30         | THR         |
| 54         | Y8           | 32         | LEU         |
| 2          | QB           | 231        | GLU         |
| 5          | QE           | 39         | GLY         |
| 11         | QK           | 115        | PRO         |
| 30         | RG           | 87         | PRO         |
| 35         | RP           | 23         | PRO         |
| 35         | RP           | 122        | PRO         |
| 41         | RV           | 79         | VAL         |
| 45         | RZ           | 141        | VAL         |
| 47         | R1           | 28         | GLY         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | YE    | 81  | ILE  |
| 35  | YP    | 11  | GLY  |
| 41  | YV    | 37  | VAL  |
| 43  | YX    | 67  | GLY  |
| 52  | Y6    | 41  | PRO  |
| 35  | RP    | 43  | GLY  |
| 35  | RP    | 97  | PRO  |
| 45  | RZ    | 108 | PRO  |
| 45  | RZ    | 139 | VAL  |
| 52  | R6    | 41  | PRO  |
| 9   | XI    | 53  | VAL  |
| 13  | XM    | 9   | ILE  |
| 28  | YE    | 52  | LEU  |
| 35  | YP    | 7   | ARG  |
| 37  | YR    | 106 | GLY  |
| 44  | YY    | 49  | VAL  |
| 3   | QC    | 51  | GLY  |
| 30  | RG    | 109 | VAL  |
| 35  | RP    | 19  | VAL  |
| 41  | RV    | 29  | PRO  |
| 45  | RZ    | 134 | PRO  |
| 50  | R4    | 22  | ILE  |
| 5   | XE    | 70  | PRO  |
| 9   | XI    | 21  | PRO  |
| 19  | XS    | 46  | GLY  |
| 20  | XT    | 97  | ALA  |
| 28  | YE    | 7   | VAL  |
| 32  | YI    | 142 | VAL  |
| 2   | QB    | 26  | PRO  |
| 28  | RE    | 7   | VAL  |
| 30  | RG    | 85  | GLY  |
| 31  | RH    | 4   | ILE  |
| 7   | XG    | 17  | VAL  |
| 9   | XI    | 28  | VAL  |
| 10  | XJ    | 37  | PRO  |
| 13  | XM    | 4   | ILE  |
| 28  | YE    | 130 | GLY  |
| 19  | QS    | 9   | VAL  |
| 35  | RP    | 146 | VAL  |
| 29  | YF    | 132 | VAL  |
| 41  | YV    | 47  | VAL  |
| 48  | R2    | 18  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | QB    | 204/220 (93%)  | 174 (85%) | 30 (15%) | 4           | 20 |
| 2   | XB    | 204/220 (93%)  | 176 (86%) | 28 (14%) | 4           | 23 |
| 3   | QC    | 160/188 (85%)  | 142 (89%) | 18 (11%) | 7           | 32 |
| 3   | XC    | 160/188 (85%)  | 142 (89%) | 18 (11%) | 7           | 32 |
| 4   | QD    | 180/181 (99%)  | 156 (87%) | 24 (13%) | 5           | 24 |
| 4   | XD    | 180/181 (99%)  | 157 (87%) | 23 (13%) | 5           | 26 |
| 5   | QE    | 119/123 (97%)  | 103 (87%) | 16 (13%) | 5           | 24 |
| 5   | XE    | 119/123 (97%)  | 106 (89%) | 13 (11%) | 8           | 34 |
| 6   | QF    | 90/90 (100%)   | 85 (94%)  | 5 (6%)   | 26          | 66 |
| 6   | XF    | 90/90 (100%)   | 76 (84%)  | 14 (16%) | 3           | 18 |
| 7   | QG    | 126/127 (99%)  | 112 (89%) | 14 (11%) | 8           | 33 |
| 7   | XG    | 126/127 (99%)  | 109 (86%) | 17 (14%) | 5           | 24 |
| 8   | QH    | 119/119 (100%) | 109 (92%) | 10 (8%)  | 14          | 49 |
| 8   | XH    | 119/119 (100%) | 106 (89%) | 13 (11%) | 8           | 34 |
| 9   | QI    | 99/99 (100%)   | 79 (80%)  | 20 (20%) | 1           | 7  |
| 9   | XI    | 99/99 (100%)   | 80 (81%)  | 19 (19%) | 2           | 9  |
| 10  | QJ    | 89/92 (97%)    | 77 (86%)  | 12 (14%) | 5           | 24 |
| 10  | XJ    | 89/92 (97%)    | 75 (84%)  | 14 (16%) | 3           | 18 |
| 11  | QK    | 92/99 (93%)    | 82 (89%)  | 10 (11%) | 8           | 34 |
| 11  | XK    | 92/99 (93%)    | 83 (90%)  | 9 (10%)  | 10          | 40 |
| 12  | QL    | 104/109 (95%)  | 89 (86%)  | 15 (14%) | 4           | 21 |
| 12  | XL    | 104/109 (95%)  | 87 (84%)  | 17 (16%) | 3           | 16 |
| 13  | QM    | 94/101 (93%)   | 80 (85%)  | 14 (15%) | 4           | 20 |
| 13  | XM    | 94/101 (93%)   | 82 (87%)  | 12 (13%) | 5           | 26 |
| 14  | QN    | 49/50 (98%)    | 48 (98%)  | 1 (2%)   | 63          | 87 |
| 14  | XN    | 49/50 (98%)    | 43 (88%)  | 6 (12%)  | 6           | 28 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 15  | QO    | 79/80 (99%)    | 74 (94%)  | 5 (6%)   | 22          | 62 |
| 15  | XO    | 79/80 (99%)    | 74 (94%)  | 5 (6%)   | 22          | 62 |
| 16  | QP    | 72/74 (97%)    | 64 (89%)  | 8 (11%)  | 8           | 33 |
| 16  | XP    | 72/74 (97%)    | 64 (89%)  | 8 (11%)  | 8           | 33 |
| 17  | QQ    | 95/97 (98%)    | 90 (95%)  | 5 (5%)   | 28          | 67 |
| 17  | XQ    | 95/97 (98%)    | 88 (93%)  | 7 (7%)   | 17          | 55 |
| 18  | QR    | 62/77 (80%)    | 56 (90%)  | 6 (10%)  | 10          | 40 |
| 18  | XR    | 62/77 (80%)    | 54 (87%)  | 8 (13%)  | 5           | 26 |
| 19  | QS    | 71/80 (89%)    | 54 (76%)  | 17 (24%) | 1           | 4  |
| 19  | XS    | 71/80 (89%)    | 58 (82%)  | 13 (18%) | 2           | 10 |
| 20  | QT    | 76/82 (93%)    | 62 (82%)  | 14 (18%) | 2           | 10 |
| 20  | XT    | 76/82 (93%)    | 66 (87%)  | 10 (13%) | 5           | 25 |
| 21  | QU    | 20/22 (91%)    | 18 (90%)  | 2 (10%)  | 9           | 38 |
| 21  | XU    | 20/22 (91%)    | 18 (90%)  | 2 (10%)  | 9           | 38 |
| 24  | QY    | 78/102 (76%)   | 75 (96%)  | 3 (4%)   | 40          | 76 |
| 24  | XY    | 78/102 (76%)   | 74 (95%)  | 4 (5%)   | 29          | 69 |
| 27  | RD    | 214/218 (98%)  | 178 (83%) | 36 (17%) | 2           | 14 |
| 27  | YD    | 214/218 (98%)  | 180 (84%) | 34 (16%) | 3           | 17 |
| 28  | RE    | 165/166 (99%)  | 137 (83%) | 28 (17%) | 2           | 14 |
| 28  | YE    | 165/166 (99%)  | 138 (84%) | 27 (16%) | 3           | 15 |
| 29  | RF    | 165/166 (99%)  | 139 (84%) | 26 (16%) | 3           | 17 |
| 29  | YF    | 165/166 (99%)  | 142 (86%) | 23 (14%) | 4           | 23 |
| 30  | RG    | 155/156 (99%)  | 148 (96%) | 7 (4%)   | 34          | 73 |
| 30  | YG    | 155/156 (99%)  | 138 (89%) | 17 (11%) | 8           | 34 |
| 31  | RH    | 142/148 (96%)  | 123 (87%) | 19 (13%) | 5           | 24 |
| 31  | YH    | 142/148 (96%)  | 117 (82%) | 25 (18%) | 2           | 12 |
| 32  | RI    | 122/124 (98%)  | 98 (80%)  | 24 (20%) | 1           | 8  |
| 32  | YI    | 122/124 (98%)  | 99 (81%)  | 23 (19%) | 2           | 9  |
| 33  | RN    | 117/119 (98%)  | 107 (92%) | 10 (8%)  | 13          | 48 |
| 33  | YN    | 117/119 (98%)  | 104 (89%) | 13 (11%) | 8           | 33 |
| 34  | RO    | 100/100 (100%) | 91 (91%)  | 9 (9%)   | 12          | 45 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 34  | YO    | 100/100 (100%) | 90 (90%)  | 10 (10%) | 9           | 38 |
| 35  | RP    | 116/116 (100%) | 83 (72%)  | 33 (28%) | 0           | 2  |
| 35  | YP    | 116/116 (100%) | 84 (72%)  | 32 (28%) | 0           | 3  |
| 36  | RQ    | 110/111 (99%)  | 93 (84%)  | 17 (16%) | 3           | 18 |
| 36  | YQ    | 110/111 (99%)  | 93 (84%)  | 17 (16%) | 3           | 18 |
| 37  | RR    | 100/101 (99%)  | 82 (82%)  | 18 (18%) | 2           | 11 |
| 37  | YR    | 100/101 (99%)  | 87 (87%)  | 13 (13%) | 5           | 25 |
| 38  | RS    | 87/88 (99%)    | 80 (92%)  | 7 (8%)   | 15          | 51 |
| 38  | YS    | 87/88 (99%)    | 73 (84%)  | 14 (16%) | 3           | 16 |
| 39  | RT    | 120/127 (94%)  | 99 (82%)  | 21 (18%) | 2           | 13 |
| 39  | YT    | 120/127 (94%)  | 98 (82%)  | 22 (18%) | 2           | 10 |
| 40  | RU    | 93/94 (99%)    | 85 (91%)  | 8 (9%)   | 13          | 48 |
| 40  | YU    | 93/94 (99%)    | 85 (91%)  | 8 (9%)   | 13          | 48 |
| 41  | RV    | 82/82 (100%)   | 65 (79%)  | 17 (21%) | 1           | 7  |
| 41  | YV    | 82/82 (100%)   | 64 (78%)  | 18 (22%) | 1           | 5  |
| 42  | RW    | 92/92 (100%)   | 82 (89%)  | 10 (11%) | 8           | 34 |
| 42  | YW    | 92/92 (100%)   | 79 (86%)  | 13 (14%) | 4           | 22 |
| 43  | RX    | 74/78 (95%)    | 65 (88%)  | 9 (12%)  | 6           | 28 |
| 43  | YX    | 74/78 (95%)    | 68 (92%)  | 6 (8%)   | 15          | 51 |
| 44  | RY    | 85/91 (93%)    | 65 (76%)  | 20 (24%) | 1           | 4  |
| 44  | YY    | 85/91 (93%)    | 61 (72%)  | 24 (28%) | 0           | 2  |
| 45  | RZ    | 155/179 (87%)  | 127 (82%) | 28 (18%) | 2           | 11 |
| 45  | YZ    | 162/179 (90%)  | 134 (83%) | 28 (17%) | 2           | 13 |
| 46  | R0    | 66/67 (98%)    | 62 (94%)  | 4 (6%)   | 23          | 63 |
| 46  | Y0    | 66/67 (98%)    | 58 (88%)  | 8 (12%)  | 6           | 28 |
| 47  | R1    | 82/83 (99%)    | 68 (83%)  | 14 (17%) | 2           | 14 |
| 47  | Y1    | 82/83 (99%)    | 72 (88%)  | 10 (12%) | 6           | 28 |
| 48  | R2    | 64/67 (96%)    | 52 (81%)  | 12 (19%) | 2           | 9  |
| 48  | Y2    | 64/67 (96%)    | 57 (89%)  | 7 (11%)  | 8           | 34 |
| 49  | R3    | 51/52 (98%)    | 44 (86%)  | 7 (14%)  | 4           | 23 |
| 49  | Y3    | 51/52 (98%)    | 47 (92%)  | 4 (8%)   | 16          | 52 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |     |
|-----|-------|------------------|------------|------------|-------------|-----|
| 50  | R4    | 62/63 (98%)      | 47 (76%)   | 15 (24%)   | 1           | 4   |
| 50  | Y4    | 62/63 (98%)      | 44 (71%)   | 18 (29%)   | 0           | 2   |
| 51  | R5    | 51/52 (98%)      | 40 (78%)   | 11 (22%)   | 1           | 6   |
| 51  | Y5    | 49/52 (94%)      | 43 (88%)   | 6 (12%)    | 6           | 28  |
| 52  | R6    | 47/52 (90%)      | 32 (68%)   | 15 (32%)   | 0           | 2   |
| 52  | Y6    | 47/52 (90%)      | 30 (64%)   | 17 (36%)   | 0           | 1   |
| 53  | R7    | 42/42 (100%)     | 35 (83%)   | 7 (17%)    | 3           | 14  |
| 53  | Y7    | 42/42 (100%)     | 35 (83%)   | 7 (17%)    | 3           | 14  |
| 54  | R8    | 54/55 (98%)      | 44 (82%)   | 10 (18%)   | 2           | 10  |
| 54  | Y8    | 54/55 (98%)      | 44 (82%)   | 10 (18%)   | 2           | 10  |
| 55  | R9    | 34/34 (100%)     | 32 (94%)   | 2 (6%)     | 24          | 64  |
| 55  | Y9    | 33/34 (97%)      | 33 (100%)  | 0          | 100         | 100 |
| All | All   | 9854/10270 (96%) | 8447 (86%) | 1407 (14%) | 4           | 22  |

All (1407) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 10  | LEU  |
| 2   | QB    | 11  | LEU  |
| 2   | QB    | 16  | HIS  |
| 2   | QB    | 17  | PHE  |
| 2   | QB    | 23  | ARG  |
| 2   | QB    | 24  | TRP  |
| 2   | QB    | 30  | ARG  |
| 2   | QB    | 31  | TYR  |
| 2   | QB    | 32  | ILE  |
| 2   | QB    | 42  | ILE  |
| 2   | QB    | 44  | LEU  |
| 2   | QB    | 80  | ILE  |
| 2   | QB    | 101 | MET  |
| 2   | QB    | 114 | ARG  |
| 2   | QB    | 135 | GLN  |
| 2   | QB    | 154 | LEU  |
| 2   | QB    | 158 | LEU  |
| 2   | QB    | 165 | VAL  |
| 2   | QB    | 178 | ARG  |
| 2   | QB    | 185 | ILE  |
| 2   | QB    | 187 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | QB    | 191 | ASP  |
| 2   | QB    | 196 | LEU  |
| 2   | QB    | 204 | ASN  |
| 2   | QB    | 208 | ILE  |
| 2   | QB    | 221 | LEU  |
| 2   | QB    | 226 | ARG  |
| 2   | QB    | 233 | SER  |
| 2   | QB    | 238 | LEU  |
| 2   | QB    | 240 | GLN  |
| 3   | QC    | 5   | ILE  |
| 3   | QC    | 16  | ARG  |
| 3   | QC    | 27  | LYS  |
| 3   | QC    | 28  | GLN  |
| 3   | QC    | 29  | TYR  |
| 3   | QC    | 36  | ASP  |
| 3   | QC    | 46  | GLU  |
| 3   | QC    | 52  | LEU  |
| 3   | QC    | 66  | VAL  |
| 3   | QC    | 75  | VAL  |
| 3   | QC    | 83  | ARG  |
| 3   | QC    | 84  | ILE  |
| 3   | QC    | 140 | ARG  |
| 3   | QC    | 161 | GLU  |
| 3   | QC    | 165 | THR  |
| 3   | QC    | 188 | LEU  |
| 3   | QC    | 196 | LEU  |
| 3   | QC    | 206 | GLU  |
| 4   | QD    | 12  | CYS  |
| 4   | QD    | 13  | ARG  |
| 4   | QD    | 19  | LEU  |
| 4   | QD    | 24  | GLU  |
| 4   | QD    | 26  | CYS  |
| 4   | QD    | 27  | TYR  |
| 4   | QD    | 31  | CYS  |
| 4   | QD    | 34  | GLU  |
| 4   | QD    | 45  | GLN  |
| 4   | QD    | 58  | LEU  |
| 4   | QD    | 84  | LYS  |
| 4   | QD    | 86  | LYS  |
| 4   | QD    | 96  | LEU  |
| 4   | QD    | 108 | LEU  |
| 4   | QD    | 119 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | QD    | 122 | ARG  |
| 4   | QD    | 127 | THR  |
| 4   | QD    | 135 | LEU  |
| 4   | QD    | 160 | GLN  |
| 4   | QD    | 178 | VAL  |
| 4   | QD    | 187 | ARG  |
| 4   | QD    | 191 | ARG  |
| 4   | QD    | 196 | LEU  |
| 4   | QD    | 200 | GLU  |
| 5   | QE    | 6   | PHE  |
| 5   | QE    | 8   | GLU  |
| 5   | QE    | 9   | LYS  |
| 5   | QE    | 25  | ARG  |
| 5   | QE    | 41  | VAL  |
| 5   | QE    | 47  | LYS  |
| 5   | QE    | 51  | VAL  |
| 5   | QE    | 60  | TYR  |
| 5   | QE    | 68  | GLU  |
| 5   | QE    | 72  | GLN  |
| 5   | QE    | 78  | HIS  |
| 5   | QE    | 79  | GLU  |
| 5   | QE    | 101 | ILE  |
| 5   | QE    | 126 | ARG  |
| 5   | QE    | 147 | ASP  |
| 5   | QE    | 152 | ARG  |
| 6   | QF    | 28  | ARG  |
| 6   | QF    | 54  | LYS  |
| 6   | QF    | 78  | GLU  |
| 6   | QF    | 83  | ASP  |
| 6   | QF    | 98  | LEU  |
| 7   | QG    | 3   | ARG  |
| 7   | QG    | 4   | ARG  |
| 7   | QG    | 8   | GLU  |
| 7   | QG    | 11  | GLN  |
| 7   | QG    | 57  | GLU  |
| 7   | QG    | 75  | VAL  |
| 7   | QG    | 78  | ARG  |
| 7   | QG    | 84  | ASN  |
| 7   | QG    | 94  | ARG  |
| 7   | QG    | 104 | LEU  |
| 7   | QG    | 136 | LYS  |
| 7   | QG    | 137 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | QG    | 151 | TYR  |
| 7   | QG    | 156 | TRP  |
| 8   | QH    | 1   | MET  |
| 8   | QH    | 25  | ASP  |
| 8   | QH    | 26  | VAL  |
| 8   | QH    | 37  | ARG  |
| 8   | QH    | 41  | ARG  |
| 8   | QH    | 56  | LYS  |
| 8   | QH    | 91  | ARG  |
| 8   | QH    | 102 | ARG  |
| 8   | QH    | 109 | ILE  |
| 8   | QH    | 137 | VAL  |
| 9   | QI    | 1   | MET  |
| 9   | QI    | 3   | GLN  |
| 9   | QI    | 10  | ARG  |
| 9   | QI    | 11  | LYS  |
| 9   | QI    | 12  | GLU  |
| 9   | QI    | 25  | LYS  |
| 9   | QI    | 38  | GLN  |
| 9   | QI    | 40  | LEU  |
| 9   | QI    | 56  | LEU  |
| 9   | QI    | 65  | VAL  |
| 9   | QI    | 88  | TYR  |
| 9   | QI    | 95  | LYS  |
| 9   | QI    | 102 | LEU  |
| 9   | QI    | 104 | ARG  |
| 9   | QI    | 110 | GLU  |
| 9   | QI    | 112 | LYS  |
| 9   | QI    | 114 | TYR  |
| 9   | QI    | 117 | HIS  |
| 9   | QI    | 121 | ARG  |
| 9   | QI    | 127 | LYS  |
| 10  | QJ    | 16  | LEU  |
| 10  | QJ    | 17  | ASP  |
| 10  | QJ    | 22  | LYS  |
| 10  | QJ    | 42  | THR  |
| 10  | QJ    | 47  | PHE  |
| 10  | QJ    | 57  | LYS  |
| 10  | QJ    | 60  | ARG  |
| 10  | QJ    | 62  | HIS  |
| 10  | QJ    | 74  | ILE  |
| 10  | QJ    | 79  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | QJ    | 80  | LYS  |
| 10  | QJ    | 96  | ILE  |
| 11  | QK    | 13  | GLN  |
| 11  | QK    | 14  | VAL  |
| 11  | QK    | 18  | ARG  |
| 11  | QK    | 29  | ILE  |
| 11  | QK    | 30  | VAL  |
| 11  | QK    | 50  | TYR  |
| 11  | QK    | 81  | ASP  |
| 11  | QK    | 84  | VAL  |
| 11  | QK    | 87  | THR  |
| 11  | QK    | 105 | VAL  |
| 12  | QL    | 8   | ASN  |
| 12  | QL    | 18  | VAL  |
| 12  | QL    | 20  | LYS  |
| 12  | QL    | 23  | LYS  |
| 12  | QL    | 24  | VAL  |
| 12  | QL    | 28  | LYS  |
| 12  | QL    | 33  | ARG  |
| 12  | QL    | 42  | THR  |
| 12  | QL    | 84  | LEU  |
| 12  | QL    | 85  | ILE  |
| 12  | QL    | 91  | LYS  |
| 12  | QL    | 92  | ASP  |
| 12  | QL    | 111 | LYS  |
| 12  | QL    | 124 | LYS  |
| 12  | QL    | 126 | LYS  |
| 13  | QM    | 9   | ILE  |
| 13  | QM    | 23  | TYR  |
| 13  | QM    | 27  | LYS  |
| 13  | QM    | 46  | LYS  |
| 13  | QM    | 48  | LEU  |
| 13  | QM    | 49  | THR  |
| 13  | QM    | 64  | TRP  |
| 13  | QM    | 66  | LEU  |
| 13  | QM    | 70  | LEU  |
| 13  | QM    | 71  | ARG  |
| 13  | QM    | 77  | ASN  |
| 13  | QM    | 81  | LEU  |
| 13  | QM    | 93  | ARG  |
| 13  | QM    | 108 | ARG  |
| 14  | QN    | 15  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | QO    | 3   | ILE  |
| 15  | QO    | 4   | THR  |
| 15  | QO    | 26  | GLU  |
| 15  | QO    | 82  | ILE  |
| 15  | QO    | 87  | ILE  |
| 16  | QP    | 18  | ARG  |
| 16  | QP    | 21  | VAL  |
| 16  | QP    | 27  | LYS  |
| 16  | QP    | 45  | THR  |
| 16  | QP    | 54  | GLU  |
| 16  | QP    | 55  | ARG  |
| 16  | QP    | 67  | THR  |
| 16  | QP    | 72  | ARG  |
| 17  | QQ    | 52  | LYS  |
| 17  | QQ    | 63  | ARG  |
| 17  | QQ    | 73  | VAL  |
| 17  | QQ    | 74  | LEU  |
| 17  | QQ    | 78  | GLU  |
| 18  | QR    | 19  | LYS  |
| 18  | QR    | 31  | LEU  |
| 18  | QR    | 58  | LEU  |
| 18  | QR    | 82  | THR  |
| 18  | QR    | 85  | LEU  |
| 18  | QR    | 87  | ARG  |
| 19  | QS    | 5   | LEU  |
| 19  | QS    | 6   | LYS  |
| 19  | QS    | 7   | LYS  |
| 19  | QS    | 10  | PHE  |
| 19  | QS    | 11  | VAL  |
| 19  | QS    | 12  | ASP  |
| 19  | QS    | 13  | ASP  |
| 19  | QS    | 19  | VAL  |
| 19  | QS    | 25  | LYS  |
| 19  | QS    | 27  | GLU  |
| 19  | QS    | 31  | ILE  |
| 19  | QS    | 34  | TRP  |
| 19  | QS    | 40  | ILE  |
| 19  | QS    | 56  | GLN  |
| 19  | QS    | 63  | THR  |
| 19  | QS    | 69  | HIS  |
| 19  | QS    | 83  | HIS  |
| 20  | QT    | 10  | LEU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 20         | QT           | 14         | LYS         |
| 20         | QT           | 24         | LEU         |
| 20         | QT           | 29         | LYS         |
| 20         | QT           | 36         | LEU         |
| 20         | QT           | 72         | LEU         |
| 20         | QT           | 73         | HIS         |
| 20         | QT           | 74         | LYS         |
| 20         | QT           | 75         | ASN         |
| 20         | QT           | 83         | ARG         |
| 20         | QT           | 84         | LEU         |
| 20         | QT           | 92         | LEU         |
| 20         | QT           | 93         | GLU         |
| 20         | QT           | 105        | SER         |
| 21         | QU           | 9          | ARG         |
| 21         | QU           | 15         | ARG         |
| 24         | QY           | 6          | LYS         |
| 24         | QY           | 48         | ARG         |
| 24         | QY           | 49         | GLN         |
| 27         | RD           | 10         | THR         |
| 27         | RD           | 20         | ASP         |
| 27         | RD           | 27         | THR         |
| 27         | RD           | 34         | VAL         |
| 27         | RD           | 43         | ARG         |
| 27         | RD           | 49         | ILE         |
| 27         | RD           | 65         | ILE         |
| 27         | RD           | 72         | LYS         |
| 27         | RD           | 94         | LEU         |
| 27         | RD           | 95         | LEU         |
| 27         | RD           | 98         | VAL         |
| 27         | RD           | 103        | ARG         |
| 27         | RD           | 104        | TYR         |
| 27         | RD           | 106        | ILE         |
| 27         | RD           | 111        | LEU         |
| 27         | RD           | 138        | VAL         |
| 27         | RD           | 150        | LYS         |
| 27         | RD           | 155        | LEU         |
| 27         | RD           | 157        | ARG         |
| 27         | RD           | 165        | ILE         |
| 27         | RD           | 166        | GLN         |
| 27         | RD           | 168        | ARG         |
| 27         | RD           | 171        | ASP         |
| 27         | RD           | 173        | VAL         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | RD    | 192 | THR  |
| 27  | RD    | 193 | VAL  |
| 27  | RD    | 211 | ARG  |
| 27  | RD    | 212 | SER  |
| 27  | RD    | 242 | ARG  |
| 27  | RD    | 244 | ARG  |
| 27  | RD    | 255 | LYS  |
| 27  | RD    | 257 | LEU  |
| 27  | RD    | 260 | ARG  |
| 27  | RD    | 268 | ARG  |
| 27  | RD    | 271 | ILE  |
| 27  | RD    | 273 | ARG  |
| 28  | RE    | 4   | ILE  |
| 28  | RE    | 37  | ARG  |
| 28  | RE    | 48  | GLN  |
| 28  | RE    | 49  | LEU  |
| 28  | RE    | 52  | LEU  |
| 28  | RE    | 54  | GLN  |
| 28  | RE    | 63  | LEU  |
| 28  | RE    | 77  | ILE  |
| 28  | RE    | 78  | LEU  |
| 28  | RE    | 82  | ARG  |
| 28  | RE    | 85  | ASN  |
| 28  | RE    | 89  | ASP  |
| 28  | RE    | 95  | ILE  |
| 28  | RE    | 113 | PHE  |
| 28  | RE    | 116 | VAL  |
| 28  | RE    | 118 | LYS  |
| 28  | RE    | 119 | ARG  |
| 28  | RE    | 134 | ILE  |
| 28  | RE    | 144 | ARG  |
| 28  | RE    | 154 | LYS  |
| 28  | RE    | 171 | GLU  |
| 28  | RE    | 179 | GLU  |
| 28  | RE    | 181 | LEU  |
| 28  | RE    | 184 | VAL  |
| 28  | RE    | 188 | VAL  |
| 28  | RE    | 197 | ILE  |
| 28  | RE    | 202 | LYS  |
| 28  | RE    | 203 | LYS  |
| 29  | RF    | 2   | LYS  |
| 29  | RF    | 7   | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | RF    | 8   | GLN  |
| 29  | RF    | 19  | GLU  |
| 29  | RF    | 20  | LEU  |
| 29  | RF    | 23  | ASP  |
| 29  | RF    | 24  | LEU  |
| 29  | RF    | 28  | ILE  |
| 29  | RF    | 33  | LEU  |
| 29  | RF    | 38  | ARG  |
| 29  | RF    | 53  | THR  |
| 29  | RF    | 57  | VAL  |
| 29  | RF    | 60  | SER  |
| 29  | RF    | 62  | ARG  |
| 29  | RF    | 70  | THR  |
| 29  | RF    | 74  | ARG  |
| 29  | RF    | 88  | VAL  |
| 29  | RF    | 96  | ASP  |
| 29  | RF    | 110 | LEU  |
| 29  | RF    | 125 | LEU  |
| 29  | RF    | 158 | THR  |
| 29  | RF    | 165 | ARG  |
| 29  | RF    | 175 | THR  |
| 29  | RF    | 183 | VAL  |
| 29  | RF    | 201 | VAL  |
| 29  | RF    | 205 | ARG  |
| 30  | RG    | 34  | LEU  |
| 30  | RG    | 63  | ILE  |
| 30  | RG    | 88  | ILE  |
| 30  | RG    | 94  | LEU  |
| 30  | RG    | 115 | ARG  |
| 30  | RG    | 133 | LEU  |
| 30  | RG    | 159 | VAL  |
| 31  | RH    | 3   | ARG  |
| 31  | RH    | 9   | ILE  |
| 31  | RH    | 17  | VAL  |
| 31  | RH    | 24  | VAL  |
| 31  | RH    | 27  | LYS  |
| 31  | RH    | 46  | GLU  |
| 31  | RH    | 49  | VAL  |
| 31  | RH    | 51  | ARG  |
| 31  | RH    | 54  | ARG  |
| 31  | RH    | 69  | ARG  |
| 31  | RH    | 83  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | RH    | 85  | LYS  |
| 31  | RH    | 89  | ILE  |
| 31  | RH    | 101 | ARG  |
| 31  | RH    | 104 | GLU  |
| 31  | RH    | 125 | VAL  |
| 31  | RH    | 130 | ARG  |
| 31  | RH    | 157 | TYR  |
| 31  | RH    | 158 | HIS  |
| 32  | RI    | 1   | MET  |
| 32  | RI    | 3   | VAL  |
| 32  | RI    | 10  | GLU  |
| 32  | RI    | 38  | LEU  |
| 32  | RI    | 56  | LYS  |
| 32  | RI    | 62  | LYS  |
| 32  | RI    | 74  | ASN  |
| 32  | RI    | 77  | LEU  |
| 32  | RI    | 81  | VAL  |
| 32  | RI    | 82  | ARG  |
| 32  | RI    | 85  | GLU  |
| 32  | RI    | 99  | GLU  |
| 32  | RI    | 101 | LEU  |
| 32  | RI    | 105 | HIS  |
| 32  | RI    | 109 | ILE  |
| 32  | RI    | 110 | ASP  |
| 32  | RI    | 114 | LEU  |
| 32  | RI    | 117 | GLU  |
| 32  | RI    | 122 | GLU  |
| 32  | RI    | 125 | GLU  |
| 32  | RI    | 130 | TYR  |
| 32  | RI    | 136 | VAL  |
| 32  | RI    | 141 | LYS  |
| 32  | RI    | 144 | VAL  |
| 33  | RN    | 1   | MET  |
| 33  | RN    | 32  | THR  |
| 33  | RN    | 43  | THR  |
| 33  | RN    | 48  | MET  |
| 33  | RN    | 56  | ASN  |
| 33  | RN    | 87  | LEU  |
| 33  | RN    | 93  | THR  |
| 33  | RN    | 94  | HIS  |
| 33  | RN    | 98  | VAL  |
| 33  | RN    | 137 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | RO    | 23  | ARG  |
| 34  | RO    | 29  | ASN  |
| 34  | RO    | 47  | ILE  |
| 34  | RO    | 49  | ARG  |
| 34  | RO    | 80  | ASP  |
| 34  | RO    | 94  | ARG  |
| 34  | RO    | 98  | VAL  |
| 34  | RO    | 108 | GLU  |
| 34  | RO    | 117 | LEU  |
| 35  | RP    | 5   | ASP  |
| 35  | RP    | 6   | LEU  |
| 35  | RP    | 9   | ASN  |
| 35  | RP    | 14  | LYS  |
| 35  | RP    | 15  | ARG  |
| 35  | RP    | 16  | ARG  |
| 35  | RP    | 19  | VAL  |
| 35  | RP    | 21  | ARG  |
| 35  | RP    | 29  | LYS  |
| 35  | RP    | 45  | LEU  |
| 35  | RP    | 52  | GLU  |
| 35  | RP    | 61  | ARG  |
| 35  | RP    | 62  | LEU  |
| 35  | RP    | 67  | MET  |
| 35  | RP    | 75  | ILE  |
| 35  | RP    | 81  | GLN  |
| 35  | RP    | 83  | VAL  |
| 35  | RP    | 98  | GLU  |
| 35  | RP    | 101 | VAL  |
| 35  | RP    | 102 | ARG  |
| 35  | RP    | 106 | LEU  |
| 35  | RP    | 110 | TYR  |
| 35  | RP    | 114 | ILE  |
| 35  | RP    | 115 | LEU  |
| 35  | RP    | 117 | GLU  |
| 35  | RP    | 125 | VAL  |
| 35  | RP    | 135 | LEU  |
| 35  | RP    | 136 | GLU  |
| 35  | RP    | 138 | LEU  |
| 35  | RP    | 144 | GLU  |
| 35  | RP    | 147 | LEU  |
| 35  | RP    | 148 | LEU  |
| 35  | RP    | 149 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | RQ    | 1   | MET  |
| 36  | RQ    | 45  | GLN  |
| 36  | RQ    | 56  | ARG  |
| 36  | RQ    | 59  | ARG  |
| 36  | RQ    | 63  | LYS  |
| 36  | RQ    | 64  | ILE  |
| 36  | RQ    | 66  | ILE  |
| 36  | RQ    | 80  | GLU  |
| 36  | RQ    | 81  | VAL  |
| 36  | RQ    | 82  | ARG  |
| 36  | RQ    | 83  | MET  |
| 36  | RQ    | 109 | VAL  |
| 36  | RQ    | 110 | THR  |
| 36  | RQ    | 112 | GLU  |
| 36  | RQ    | 113 | GLN  |
| 36  | RQ    | 115 | MET  |
| 36  | RQ    | 134 | ARG  |
| 37  | RR    | 2   | ARG  |
| 37  | RR    | 4   | LEU  |
| 37  | RR    | 6   | SER  |
| 37  | RR    | 9   | LYS  |
| 37  | RR    | 15  | SER  |
| 37  | RR    | 17  | ARG  |
| 37  | RR    | 28  | LEU  |
| 37  | RR    | 29  | LEU  |
| 37  | RR    | 37  | THR  |
| 37  | RR    | 54  | LEU  |
| 37  | RR    | 65  | LEU  |
| 37  | RR    | 67  | LEU  |
| 37  | RR    | 71  | GLN  |
| 37  | RR    | 76  | VAL  |
| 37  | RR    | 79  | LEU  |
| 37  | RR    | 99  | LYS  |
| 37  | RR    | 104 | ARG  |
| 37  | RR    | 105 | ARG  |
| 38  | RS    | 4   | LEU  |
| 38  | RS    | 20  | ARG  |
| 38  | RS    | 52  | SER  |
| 38  | RS    | 56  | LEU  |
| 38  | RS    | 98  | VAL  |
| 38  | RS    | 106 | ARG  |
| 38  | RS    | 110 | LEU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 39         | RT           | 8          | LYS         |
| 39         | RT           | 9          | LEU         |
| 39         | RT           | 23         | ARG         |
| 39         | RT           | 27         | THR         |
| 39         | RT           | 29         | ARG         |
| 39         | RT           | 30         | VAL         |
| 39         | RT           | 35         | LYS         |
| 39         | RT           | 41         | ARG         |
| 39         | RT           | 50         | ILE         |
| 39         | RT           | 58         | ASN         |
| 39         | RT           | 59         | THR         |
| 39         | RT           | 74         | ARG         |
| 39         | RT           | 78         | LEU         |
| 39         | RT           | 86         | ILE         |
| 39         | RT           | 87         | ASP         |
| 39         | RT           | 88         | ILE         |
| 39         | RT           | 93         | ARG         |
| 39         | RT           | 95         | ARG         |
| 39         | RT           | 98         | LYS         |
| 39         | RT           | 99         | LEU         |
| 39         | RT           | 137        | LYS         |
| 40         | RU           | 31         | SER         |
| 40         | RU           | 37         | GLU         |
| 40         | RU           | 74         | LEU         |
| 40         | RU           | 83         | LEU         |
| 40         | RU           | 92         | ARG         |
| 40         | RU           | 104        | GLN         |
| 40         | RU           | 114        | LYS         |
| 40         | RU           | 117        | GLN         |
| 41         | RV           | 5          | VAL         |
| 41         | RV           | 15         | GLU         |
| 41         | RV           | 19         | LYS         |
| 41         | RV           | 22         | VAL         |
| 41         | RV           | 32         | THR         |
| 41         | RV           | 35         | LEU         |
| 41         | RV           | 47         | VAL         |
| 41         | RV           | 66         | ARG         |
| 41         | RV           | 70         | ILE         |
| 41         | RV           | 76         | LYS         |
| 41         | RV           | 78         | LYS         |
| 41         | RV           | 79         | VAL         |
| 41         | RV           | 80         | GLN         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 41         | RV           | 81         | TYR         |
| 41         | RV           | 87         | HIS         |
| 41         | RV           | 95         | LEU         |
| 41         | RV           | 98         | GLU         |
| 42         | RW           | 11         | ARG         |
| 42         | RW           | 17         | VAL         |
| 42         | RW           | 69         | LEU         |
| 42         | RW           | 76         | VAL         |
| 42         | RW           | 88         | ARG         |
| 42         | RW           | 96         | ILE         |
| 42         | RW           | 100        | THR         |
| 42         | RW           | 106        | ILE         |
| 42         | RW           | 107        | LEU         |
| 42         | RW           | 113        | LYS         |
| 43         | RX           | 14         | SER         |
| 43         | RX           | 27         | THR         |
| 43         | RX           | 36         | LYS         |
| 43         | RX           | 48         | LYS         |
| 43         | RX           | 50         | LYS         |
| 43         | RX           | 63         | LYS         |
| 43         | RX           | 66         | LEU         |
| 43         | RX           | 76         | ARG         |
| 43         | RX           | 80         | ILE         |
| 44         | RY           | 5          | MET         |
| 44         | RY           | 9          | LYS         |
| 44         | RY           | 14         | LEU         |
| 44         | RY           | 17         | SER         |
| 44         | RY           | 19         | LYS         |
| 44         | RY           | 28         | LYS         |
| 44         | RY           | 33         | LYS         |
| 44         | RY           | 38         | ILE         |
| 44         | RY           | 50         | ARG         |
| 44         | RY           | 55         | TYR         |
| 44         | RY           | 60         | PHE         |
| 44         | RY           | 61         | ILE         |
| 44         | RY           | 62         | GLU         |
| 44         | RY           | 63         | LYS         |
| 44         | RY           | 86         | ARG         |
| 44         | RY           | 89         | PHE         |
| 44         | RY           | 95         | LYS         |
| 44         | RY           | 96         | ILE         |
| 44         | RY           | 97         | ARG         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 44         | RY           | 102        | CYS         |
| 45         | RZ           | 4          | ARG         |
| 45         | RZ           | 5          | LEU         |
| 45         | RZ           | 33         | LEU         |
| 45         | RZ           | 60         | GLU         |
| 45         | RZ           | 61         | LEU         |
| 45         | RZ           | 70         | LEU         |
| 45         | RZ           | 76         | LEU         |
| 45         | RZ           | 81         | ARG         |
| 45         | RZ           | 87         | ASP         |
| 45         | RZ           | 91         | LEU         |
| 45         | RZ           | 92         | SER         |
| 45         | RZ           | 104        | PHE         |
| 45         | RZ           | 112        | ARG         |
| 45         | RZ           | 118        | GLN         |
| 45         | RZ           | 120        | ILE         |
| 45         | RZ           | 121        | HIS         |
| 45         | RZ           | 128        | VAL         |
| 45         | RZ           | 135        | GLU         |
| 45         | RZ           | 136        | PHE         |
| 45         | RZ           | 138        | GLU         |
| 45         | RZ           | 140        | ASP         |
| 45         | RZ           | 141        | VAL         |
| 45         | RZ           | 144        | LEU         |
| 45         | RZ           | 148        | ASP         |
| 45         | RZ           | 156        | LYS         |
| 45         | RZ           | 157        | LEU         |
| 45         | RZ           | 171        | ILE         |
| 45         | RZ           | 175        | VAL         |
| 46         | R0           | 3          | HIS         |
| 46         | R0           | 20         | ARG         |
| 46         | R0           | 36         | ILE         |
| 46         | R0           | 53         | MET         |
| 47         | R1           | 3          | LYS         |
| 47         | R1           | 4          | VAL         |
| 47         | R1           | 38         | SER         |
| 47         | R1           | 40         | ARG         |
| 47         | R1           | 41         | ARG         |
| 47         | R1           | 57         | GLU         |
| 47         | R1           | 78         | LYS         |
| 47         | R1           | 80         | LEU         |
| 47         | R1           | 81         | LYS         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | R1    | 82  | LEU  |
| 47  | R1    | 90  | ILE  |
| 47  | R1    | 94  | LEU  |
| 47  | R1    | 97  | LEU  |
| 47  | R1    | 98  | LEU  |
| 48  | R2    | 4   | SER  |
| 48  | R2    | 24  | LEU  |
| 48  | R2    | 25  | VAL  |
| 48  | R2    | 35  | LEU  |
| 48  | R2    | 47  | ASN  |
| 48  | R2    | 48  | HIS  |
| 48  | R2    | 50  | ILE  |
| 48  | R2    | 53  | LEU  |
| 48  | R2    | 57  | ILE  |
| 48  | R2    | 60  | LEU  |
| 48  | R2    | 62  | THR  |
| 48  | R2    | 67  | LYS  |
| 49  | R3    | 8   | LEU  |
| 49  | R3    | 24  | LYS  |
| 49  | R3    | 31  | LEU  |
| 49  | R3    | 32  | GLN  |
| 49  | R3    | 40  | THR  |
| 49  | R3    | 54  | VAL  |
| 49  | R3    | 56  | VAL  |
| 50  | R4    | 8   | LYS  |
| 50  | R4    | 10  | VAL  |
| 50  | R4    | 16  | CYS  |
| 50  | R4    | 21  | VAL  |
| 50  | R4    | 31  | ILE  |
| 50  | R4    | 34  | GLU  |
| 50  | R4    | 35  | VAL  |
| 50  | R4    | 43  | TYR  |
| 50  | R4    | 50  | VAL  |
| 50  | R4    | 55  | ARG  |
| 50  | R4    | 59  | PHE  |
| 50  | R4    | 61  | ARG  |
| 50  | R4    | 63  | TYR  |
| 50  | R4    | 67  | TYR  |
| 50  | R4    | 69  | LYS  |
| 51  | R5    | 3   | LYS  |
| 51  | R5    | 4   | HIS  |
| 51  | R5    | 6   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | R5    | 11  | THR  |
| 51  | R5    | 23  | HIS  |
| 51  | R5    | 26  | THR  |
| 51  | R5    | 36  | CYS  |
| 51  | R5    | 48  | GLU  |
| 51  | R5    | 49  | CYS  |
| 51  | R5    | 51  | TYR  |
| 51  | R5    | 52  | TYR  |
| 52  | R6    | 7   | ILE  |
| 52  | R6    | 8   | LYS  |
| 52  | R6    | 10  | LEU  |
| 52  | R6    | 12  | GLU  |
| 52  | R6    | 16  | CYS  |
| 52  | R6    | 21  | TYR  |
| 52  | R6    | 24  | GLU  |
| 52  | R6    | 28  | ARG  |
| 52  | R6    | 30  | THR  |
| 52  | R6    | 33  | LYS  |
| 52  | R6    | 37  | ARG  |
| 52  | R6    | 38  | LYS  |
| 52  | R6    | 39  | TYR  |
| 52  | R6    | 45  | LYS  |
| 52  | R6    | 47  | THR  |
| 53  | R7    | 1   | MET  |
| 53  | R7    | 12  | ARG  |
| 53  | R7    | 24  | THR  |
| 53  | R7    | 43  | THR  |
| 53  | R7    | 47  | ARG  |
| 53  | R7    | 48  | LYS  |
| 53  | R7    | 49  | ARG  |
| 54  | R8    | 14  | VAL  |
| 54  | R8    | 32  | LEU  |
| 54  | R8    | 33  | ASN  |
| 54  | R8    | 40  | GLU  |
| 54  | R8    | 41  | ILE  |
| 54  | R8    | 52  | LYS  |
| 54  | R8    | 54  | GLU  |
| 54  | R8    | 58  | ILE  |
| 54  | R8    | 61  | LEU  |
| 54  | R8    | 64  | TYR  |
| 55  | R9    | 1   | MET  |
| 55  | R9    | 17  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | XB    | 11  | LEU  |
| 2   | XB    | 17  | PHE  |
| 2   | XB    | 23  | ARG  |
| 2   | XB    | 24  | TRP  |
| 2   | XB    | 30  | ARG  |
| 2   | XB    | 31  | TYR  |
| 2   | XB    | 37  | ASN  |
| 2   | XB    | 42  | ILE  |
| 2   | XB    | 44  | LEU  |
| 2   | XB    | 49  | GLU  |
| 2   | XB    | 69  | LEU  |
| 2   | XB    | 108 | ILE  |
| 2   | XB    | 114 | ARG  |
| 2   | XB    | 122 | PHE  |
| 2   | XB    | 127 | ILE  |
| 2   | XB    | 144 | ARG  |
| 2   | XB    | 145 | LEU  |
| 2   | XB    | 153 | ARG  |
| 2   | XB    | 154 | LEU  |
| 2   | XB    | 156 | LYS  |
| 2   | XB    | 165 | VAL  |
| 2   | XB    | 185 | ILE  |
| 2   | XB    | 196 | LEU  |
| 2   | XB    | 208 | ILE  |
| 2   | XB    | 209 | ARG  |
| 2   | XB    | 226 | ARG  |
| 2   | XB    | 238 | LEU  |
| 2   | XB    | 240 | GLN  |
| 3   | XC    | 5   | ILE  |
| 3   | XC    | 27  | LYS  |
| 3   | XC    | 36  | ASP  |
| 3   | XC    | 46  | GLU  |
| 3   | XC    | 66  | VAL  |
| 3   | XC    | 75  | VAL  |
| 3   | XC    | 83  | ARG  |
| 3   | XC    | 84  | ILE  |
| 3   | XC    | 94  | LEU  |
| 3   | XC    | 108 | ASN  |
| 3   | XC    | 119 | ARG  |
| 3   | XC    | 131 | ARG  |
| 3   | XC    | 140 | ARG  |
| 3   | XC    | 143 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | XC    | 161 | GLU  |
| 3   | XC    | 188 | LEU  |
| 3   | XC    | 196 | LEU  |
| 3   | XC    | 204 | LEU  |
| 4   | XD    | 8   | VAL  |
| 4   | XD    | 10  | ARG  |
| 4   | XD    | 14  | ARG  |
| 4   | XD    | 18  | LYS  |
| 4   | XD    | 19  | LEU  |
| 4   | XD    | 24  | GLU  |
| 4   | XD    | 31  | CYS  |
| 4   | XD    | 45  | GLN  |
| 4   | XD    | 58  | LEU  |
| 4   | XD    | 76  | ARG  |
| 4   | XD    | 84  | LYS  |
| 4   | XD    | 86  | LYS  |
| 4   | XD    | 96  | LEU  |
| 4   | XD    | 122 | ARG  |
| 4   | XD    | 127 | THR  |
| 4   | XD    | 135 | LEU  |
| 4   | XD    | 163 | GLU  |
| 4   | XD    | 168 | ARG  |
| 4   | XD    | 170 | VAL  |
| 4   | XD    | 187 | ARG  |
| 4   | XD    | 191 | ARG  |
| 4   | XD    | 194 | LEU  |
| 4   | XD    | 199 | ASN  |
| 5   | XE    | 6   | PHE  |
| 5   | XE    | 9   | LYS  |
| 5   | XE    | 12  | LEU  |
| 5   | XE    | 13  | ILE  |
| 5   | XE    | 41  | VAL  |
| 5   | XE    | 47  | LYS  |
| 5   | XE    | 51  | VAL  |
| 5   | XE    | 60  | TYR  |
| 5   | XE    | 72  | GLN  |
| 5   | XE    | 78  | HIS  |
| 5   | XE    | 79  | GLU  |
| 5   | XE    | 101 | ILE  |
| 5   | XE    | 155 | GLU  |
| 6   | XF    | 3   | ARG  |
| 6   | XF    | 7   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | XF    | 15  | ASP  |
| 6   | XF    | 16  | GLN  |
| 6   | XF    | 21  | LEU  |
| 6   | XF    | 28  | ARG  |
| 6   | XF    | 38  | GLU  |
| 6   | XF    | 55  | ASP  |
| 6   | XF    | 64  | GLN  |
| 6   | XF    | 70  | ASP  |
| 6   | XF    | 72  | VAL  |
| 6   | XF    | 83  | ASP  |
| 6   | XF    | 85  | VAL  |
| 6   | XF    | 98  | LEU  |
| 7   | XG    | 3   | ARG  |
| 7   | XG    | 8   | GLU  |
| 7   | XG    | 16  | LEU  |
| 7   | XG    | 21  | VAL  |
| 7   | XG    | 78  | ARG  |
| 7   | XG    | 80  | VAL  |
| 7   | XG    | 84  | ASN  |
| 7   | XG    | 97  | GLN  |
| 7   | XG    | 104 | LEU  |
| 7   | XG    | 113 | GLU  |
| 7   | XG    | 114 | ARG  |
| 7   | XG    | 118 | VAL  |
| 7   | XG    | 136 | LYS  |
| 7   | XG    | 137 | LYS  |
| 7   | XG    | 151 | TYR  |
| 7   | XG    | 155 | ARG  |
| 7   | XG    | 156 | TRP  |
| 8   | XH    | 1   | MET  |
| 8   | XH    | 3   | THR  |
| 8   | XH    | 23  | SER  |
| 8   | XH    | 24  | THR  |
| 8   | XH    | 25  | ASP  |
| 8   | XH    | 26  | VAL  |
| 8   | XH    | 37  | ARG  |
| 8   | XH    | 41  | ARG  |
| 8   | XH    | 56  | LYS  |
| 8   | XH    | 60  | ARG  |
| 8   | XH    | 102 | ARG  |
| 8   | XH    | 112 | LEU  |
| 8   | XH    | 133 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | XI    | 1   | MET  |
| 9   | XI    | 10  | ARG  |
| 9   | XI    | 25  | LYS  |
| 9   | XI    | 31  | GLN  |
| 9   | XI    | 35  | GLU  |
| 9   | XI    | 38  | GLN  |
| 9   | XI    | 47  | LEU  |
| 9   | XI    | 56  | LEU  |
| 9   | XI    | 60  | ASP  |
| 9   | XI    | 70  | LYS  |
| 9   | XI    | 88  | TYR  |
| 9   | XI    | 95  | LYS  |
| 9   | XI    | 96  | LEU  |
| 9   | XI    | 102 | LEU  |
| 9   | XI    | 104 | ARG  |
| 9   | XI    | 114 | TYR  |
| 9   | XI    | 117 | HIS  |
| 9   | XI    | 121 | ARG  |
| 9   | XI    | 125 | TYR  |
| 10  | XJ    | 16  | LEU  |
| 10  | XJ    | 17  | ASP  |
| 10  | XJ    | 22  | LYS  |
| 10  | XJ    | 40  | LEU  |
| 10  | XJ    | 47  | PHE  |
| 10  | XJ    | 62  | HIS  |
| 10  | XJ    | 70  | ARG  |
| 10  | XJ    | 74  | ILE  |
| 10  | XJ    | 78  | ASN  |
| 10  | XJ    | 79  | ARG  |
| 10  | XJ    | 80  | LYS  |
| 10  | XJ    | 96  | ILE  |
| 10  | XJ    | 97  | GLU  |
| 10  | XJ    | 98  | ILE  |
| 11  | XK    | 13  | GLN  |
| 11  | XK    | 14  | VAL  |
| 11  | XK    | 18  | ARG  |
| 11  | XK    | 29  | ILE  |
| 11  | XK    | 30  | VAL  |
| 11  | XK    | 54  | ARG  |
| 11  | XK    | 84  | VAL  |
| 11  | XK    | 114 | VAL  |
| 11  | XK    | 120 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | XL    | 18  | VAL  |
| 12  | XL    | 20  | LYS  |
| 12  | XL    | 23  | LYS  |
| 12  | XL    | 24  | VAL  |
| 12  | XL    | 27  | LEU  |
| 12  | XL    | 28  | LYS  |
| 12  | XL    | 33  | ARG  |
| 12  | XL    | 42  | THR  |
| 12  | XL    | 54  | LYS  |
| 12  | XL    | 62  | SER  |
| 12  | XL    | 83  | VAL  |
| 12  | XL    | 84  | LEU  |
| 12  | XL    | 85  | ILE  |
| 12  | XL    | 111 | LYS  |
| 12  | XL    | 116 | SER  |
| 12  | XL    | 124 | LYS  |
| 12  | XL    | 126 | LYS  |
| 13  | XM    | 4   | ILE  |
| 13  | XM    | 14  | ARG  |
| 13  | XM    | 35  | GLU  |
| 13  | XM    | 47  | ASP  |
| 13  | XM    | 48  | LEU  |
| 13  | XM    | 56  | LEU  |
| 13  | XM    | 64  | TRP  |
| 13  | XM    | 66  | LEU  |
| 13  | XM    | 70  | LEU  |
| 13  | XM    | 93  | ARG  |
| 13  | XM    | 99  | ARG  |
| 13  | XM    | 108 | ARG  |
| 14  | XN    | 15  | LYS  |
| 14  | XN    | 18  | VAL  |
| 14  | XN    | 26  | ARG  |
| 14  | XN    | 32  | SER  |
| 14  | XN    | 41  | ARG  |
| 14  | XN    | 58  | LYS  |
| 15  | XO    | 3   | ILE  |
| 15  | XO    | 39  | LEU  |
| 15  | XO    | 82  | ILE  |
| 15  | XO    | 84  | LYS  |
| 15  | XO    | 87  | ILE  |
| 16  | XP    | 2   | VAL  |
| 16  | XP    | 21  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | XP    | 27  | LYS  |
| 16  | XP    | 45  | THR  |
| 16  | XP    | 53  | VAL  |
| 16  | XP    | 54  | GLU  |
| 16  | XP    | 67  | THR  |
| 16  | XP    | 82  | GLN  |
| 17  | XQ    | 52  | LYS  |
| 17  | XQ    | 63  | ARG  |
| 17  | XQ    | 65  | ILE  |
| 17  | XQ    | 73  | VAL  |
| 17  | XQ    | 74  | LEU  |
| 17  | XQ    | 81  | ARG  |
| 17  | XQ    | 92  | ARG  |
| 18  | XR    | 19  | LYS  |
| 18  | XR    | 28  | GLU  |
| 18  | XR    | 31  | LEU  |
| 18  | XR    | 37  | VAL  |
| 18  | XR    | 58  | LEU  |
| 18  | XR    | 82  | THR  |
| 18  | XR    | 85  | LEU  |
| 18  | XR    | 87  | ARG  |
| 19  | XS    | 5   | LEU  |
| 19  | XS    | 6   | LYS  |
| 19  | XS    | 7   | LYS  |
| 19  | XS    | 10  | PHE  |
| 19  | XS    | 19  | VAL  |
| 19  | XS    | 25  | LYS  |
| 19  | XS    | 27  | GLU  |
| 19  | XS    | 31  | ILE  |
| 19  | XS    | 32  | LYS  |
| 19  | XS    | 34  | TRP  |
| 19  | XS    | 40  | ILE  |
| 19  | XS    | 60  | VAL  |
| 19  | XS    | 64  | GLU  |
| 20  | XT    | 10  | LEU  |
| 20  | XT    | 14  | LYS  |
| 20  | XT    | 35  | THR  |
| 20  | XT    | 72  | LEU  |
| 20  | XT    | 73  | HIS  |
| 20  | XT    | 74  | LYS  |
| 20  | XT    | 75  | ASN  |
| 20  | XT    | 81  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | XT    | 84  | LEU  |
| 20  | XT    | 93  | GLU  |
| 21  | XU    | 9   | ARG  |
| 21  | XU    | 15  | ARG  |
| 24  | XY    | 26  | ASP  |
| 24  | XY    | 47  | ASN  |
| 24  | XY    | 85  | ILE  |
| 24  | XY    | 91  | TYR  |
| 27  | YD    | 18  | VAL  |
| 27  | YD    | 24  | ILE  |
| 27  | YD    | 25  | THR  |
| 27  | YD    | 33  | LEU  |
| 27  | YD    | 34  | VAL  |
| 27  | YD    | 43  | ARG  |
| 27  | YD    | 44  | ASN  |
| 27  | YD    | 61  | LEU  |
| 27  | YD    | 65  | ILE  |
| 27  | YD    | 71  | ASP  |
| 27  | YD    | 75  | ILE  |
| 27  | YD    | 88  | ARG  |
| 27  | YD    | 92  | ILE  |
| 27  | YD    | 94  | LEU  |
| 27  | YD    | 95  | LEU  |
| 27  | YD    | 103 | ARG  |
| 27  | YD    | 104 | TYR  |
| 27  | YD    | 106 | ILE  |
| 27  | YD    | 111 | LEU  |
| 27  | YD    | 142 | VAL  |
| 27  | YD    | 150 | LYS  |
| 27  | YD    | 154 | LYS  |
| 27  | YD    | 157 | ARG  |
| 27  | YD    | 166 | GLN  |
| 27  | YD    | 168 | ARG  |
| 27  | YD    | 192 | THR  |
| 27  | YD    | 193 | VAL  |
| 27  | YD    | 211 | ARG  |
| 27  | YD    | 242 | ARG  |
| 27  | YD    | 244 | ARG  |
| 27  | YD    | 257 | LEU  |
| 27  | YD    | 268 | ARG  |
| 27  | YD    | 271 | ILE  |
| 27  | YD    | 273 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | YE    | 4   | ILE  |
| 28  | YE    | 12  | THR  |
| 28  | YE    | 35  | GLN  |
| 28  | YE    | 37  | ARG  |
| 28  | YE    | 47  | VAL  |
| 28  | YE    | 63  | LEU  |
| 28  | YE    | 66  | HIS  |
| 28  | YE    | 75  | VAL  |
| 28  | YE    | 78  | LEU  |
| 28  | YE    | 79  | ARG  |
| 28  | YE    | 82  | ARG  |
| 28  | YE    | 111 | ARG  |
| 28  | YE    | 116 | VAL  |
| 28  | YE    | 118 | LYS  |
| 28  | YE    | 119 | ARG  |
| 28  | YE    | 134 | ILE  |
| 28  | YE    | 144 | ARG  |
| 28  | YE    | 152 | LYS  |
| 28  | YE    | 154 | LYS  |
| 28  | YE    | 179 | GLU  |
| 28  | YE    | 181 | LEU  |
| 28  | YE    | 184 | VAL  |
| 28  | YE    | 185 | LYS  |
| 28  | YE    | 188 | VAL  |
| 28  | YE    | 201 | THR  |
| 28  | YE    | 202 | LYS  |
| 28  | YE    | 203 | LYS  |
| 29  | YF    | 2   | LYS  |
| 29  | YF    | 6   | VAL  |
| 29  | YF    | 7   | TYR  |
| 29  | YF    | 8   | GLN  |
| 29  | YF    | 20  | LEU  |
| 29  | YF    | 24  | LEU  |
| 29  | YF    | 33  | LEU  |
| 29  | YF    | 45  | ARG  |
| 29  | YF    | 53  | THR  |
| 29  | YF    | 57  | VAL  |
| 29  | YF    | 60  | SER  |
| 29  | YF    | 74  | ARG  |
| 29  | YF    | 83  | PHE  |
| 29  | YF    | 88  | VAL  |
| 29  | YF    | 110 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | YF    | 125 | LEU  |
| 29  | YF    | 136 | THR  |
| 29  | YF    | 140 | LEU  |
| 29  | YF    | 153 | SER  |
| 29  | YF    | 158 | THR  |
| 29  | YF    | 164 | ARG  |
| 29  | YF    | 183 | VAL  |
| 29  | YF    | 192 | LEU  |
| 30  | YG    | 4   | ASP  |
| 30  | YG    | 7   | LEU  |
| 30  | YG    | 26  | GLN  |
| 30  | YG    | 34  | LEU  |
| 30  | YG    | 35  | GLU  |
| 30  | YG    | 38  | VAL  |
| 30  | YG    | 60  | LEU  |
| 30  | YG    | 79  | ASN  |
| 30  | YG    | 80  | PHE  |
| 30  | YG    | 88  | ILE  |
| 30  | YG    | 101 | ILE  |
| 30  | YG    | 113 | ARG  |
| 30  | YG    | 114 | ILE  |
| 30  | YG    | 118 | ARG  |
| 30  | YG    | 123 | ASN  |
| 30  | YG    | 159 | VAL  |
| 30  | YG    | 164 | GLU  |
| 31  | YH    | 9   | ILE  |
| 31  | YH    | 17  | VAL  |
| 31  | YH    | 27  | LYS  |
| 31  | YH    | 32  | GLU  |
| 31  | YH    | 34  | GLU  |
| 31  | YH    | 45  | VAL  |
| 31  | YH    | 49  | VAL  |
| 31  | YH    | 51  | ARG  |
| 31  | YH    | 54  | ARG  |
| 31  | YH    | 59  | ARG  |
| 31  | YH    | 77  | LYS  |
| 31  | YH    | 85  | LYS  |
| 31  | YH    | 89  | ILE  |
| 31  | YH    | 103 | LEU  |
| 31  | YH    | 105 | LEU  |
| 31  | YH    | 106 | THR  |
| 31  | YH    | 107 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | YH    | 109 | PHE  |
| 31  | YH    | 125 | VAL  |
| 31  | YH    | 130 | ARG  |
| 31  | YH    | 136 | ILE  |
| 31  | YH    | 143 | GLN  |
| 31  | YH    | 157 | TYR  |
| 31  | YH    | 158 | HIS  |
| 31  | YH    | 167 | GLU  |
| 32  | YI    | 1   | MET  |
| 32  | YI    | 2   | LYS  |
| 32  | YI    | 5   | LEU  |
| 32  | YI    | 9   | LEU  |
| 32  | YI    | 20  | ASP  |
| 32  | YI    | 38  | LEU  |
| 32  | YI    | 40  | THR  |
| 32  | YI    | 52  | ARG  |
| 32  | YI    | 54  | GLN  |
| 32  | YI    | 56  | LYS  |
| 32  | YI    | 62  | LYS  |
| 32  | YI    | 74  | ASN  |
| 32  | YI    | 77  | LEU  |
| 32  | YI    | 81  | VAL  |
| 32  | YI    | 87  | LYS  |
| 32  | YI    | 101 | LEU  |
| 32  | YI    | 105 | HIS  |
| 32  | YI    | 109 | ILE  |
| 32  | YI    | 114 | LEU  |
| 32  | YI    | 117 | GLU  |
| 32  | YI    | 122 | GLU  |
| 32  | YI    | 130 | TYR  |
| 32  | YI    | 141 | LYS  |
| 33  | YN    | 1   | MET  |
| 33  | YN    | 14  | VAL  |
| 33  | YN    | 41  | ASP  |
| 33  | YN    | 48  | MET  |
| 33  | YN    | 67  | LEU  |
| 33  | YN    | 87  | LEU  |
| 33  | YN    | 88  | GLU  |
| 33  | YN    | 93  | THR  |
| 33  | YN    | 94  | HIS  |
| 33  | YN    | 99  | LEU  |
| 33  | YN    | 120 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | YN    | 127 | ASP  |
| 33  | YN    | 137 | LYS  |
| 34  | YO    | 1   | MET  |
| 34  | YO    | 29  | ASN  |
| 34  | YO    | 47  | ILE  |
| 34  | YO    | 48  | PRO  |
| 34  | YO    | 49  | ARG  |
| 34  | YO    | 73  | ASP  |
| 34  | YO    | 80  | ASP  |
| 34  | YO    | 97  | ARG  |
| 34  | YO    | 108 | GLU  |
| 34  | YO    | 117 | LEU  |
| 35  | YP    | 5   | ASP  |
| 35  | YP    | 6   | LEU  |
| 35  | YP    | 9   | ASN  |
| 35  | YP    | 14  | LYS  |
| 35  | YP    | 15  | ARG  |
| 35  | YP    | 19  | VAL  |
| 35  | YP    | 21  | ARG  |
| 35  | YP    | 27  | HIS  |
| 35  | YP    | 40  | SER  |
| 35  | YP    | 45  | LEU  |
| 35  | YP    | 52  | GLU  |
| 35  | YP    | 56  | SER  |
| 35  | YP    | 58  | THR  |
| 35  | YP    | 59  | LEU  |
| 35  | YP    | 61  | ARG  |
| 35  | YP    | 62  | LEU  |
| 35  | YP    | 75  | ILE  |
| 35  | YP    | 81  | GLN  |
| 35  | YP    | 85  | LEU  |
| 35  | YP    | 87  | ASP  |
| 35  | YP    | 98  | GLU  |
| 35  | YP    | 110 | TYR  |
| 35  | YP    | 112 | LEU  |
| 35  | YP    | 114 | ILE  |
| 35  | YP    | 115 | LEU  |
| 35  | YP    | 117 | GLU  |
| 35  | YP    | 136 | GLU  |
| 35  | YP    | 138 | LEU  |
| 35  | YP    | 144 | GLU  |
| 35  | YP    | 147 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | YP    | 148 | LEU  |
| 35  | YP    | 149 | GLU  |
| 36  | YQ    | 1   | MET  |
| 36  | YQ    | 10  | ARG  |
| 36  | YQ    | 27  | VAL  |
| 36  | YQ    | 45  | GLN  |
| 36  | YQ    | 52  | VAL  |
| 36  | YQ    | 56  | ARG  |
| 36  | YQ    | 64  | ILE  |
| 36  | YQ    | 66  | ILE  |
| 36  | YQ    | 79  | LEU  |
| 36  | YQ    | 80  | GLU  |
| 36  | YQ    | 81  | VAL  |
| 36  | YQ    | 82  | ARG  |
| 36  | YQ    | 83  | MET  |
| 36  | YQ    | 102 | VAL  |
| 36  | YQ    | 103 | MET  |
| 36  | YQ    | 134 | ARG  |
| 36  | YQ    | 138 | ASP  |
| 37  | YR    | 6   | SER  |
| 37  | YR    | 15  | SER  |
| 37  | YR    | 18  | LEU  |
| 37  | YR    | 28  | LEU  |
| 37  | YR    | 29  | LEU  |
| 37  | YR    | 67  | LEU  |
| 37  | YR    | 74  | LYS  |
| 37  | YR    | 76  | VAL  |
| 37  | YR    | 79  | LEU  |
| 37  | YR    | 81  | ASP  |
| 37  | YR    | 104 | ARG  |
| 37  | YR    | 113 | LEU  |
| 37  | YR    | 117 | VAL  |
| 38  | YS    | 12  | PHE  |
| 38  | YS    | 20  | ARG  |
| 38  | YS    | 27  | SER  |
| 38  | YS    | 49  | VAL  |
| 38  | YS    | 52  | SER  |
| 38  | YS    | 54  | LEU  |
| 38  | YS    | 56  | LEU  |
| 38  | YS    | 58  | LEU  |
| 38  | YS    | 59  | LYS  |
| 38  | YS    | 69  | VAL  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 38         | YS           | 73         | LEU         |
| 38         | YS           | 89         | ARG         |
| 38         | YS           | 106        | ARG         |
| 38         | YS           | 110        | LEU         |
| 39         | YT           | 8          | LYS         |
| 39         | YT           | 23         | ARG         |
| 39         | YT           | 28         | VAL         |
| 39         | YT           | 30         | VAL         |
| 39         | YT           | 33         | LYS         |
| 39         | YT           | 35         | LYS         |
| 39         | YT           | 41         | ARG         |
| 39         | YT           | 50         | ILE         |
| 39         | YT           | 58         | ASN         |
| 39         | YT           | 59         | THR         |
| 39         | YT           | 62         | THR         |
| 39         | YT           | 74         | ARG         |
| 39         | YT           | 78         | LEU         |
| 39         | YT           | 88         | ILE         |
| 39         | YT           | 89         | VAL         |
| 39         | YT           | 91         | ARG         |
| 39         | YT           | 98         | LYS         |
| 39         | YT           | 99         | LEU         |
| 39         | YT           | 102        | ILE         |
| 39         | YT           | 107        | ASP         |
| 39         | YT           | 115        | ARG         |
| 39         | YT           | 137        | LYS         |
| 40         | YU           | 5          | LYS         |
| 40         | YU           | 27         | LEU         |
| 40         | YU           | 74         | LEU         |
| 40         | YU           | 88         | ILE         |
| 40         | YU           | 92         | ARG         |
| 40         | YU           | 93         | LYS         |
| 40         | YU           | 97         | ASP         |
| 40         | YU           | 114        | LYS         |
| 41         | YV           | 2          | PHE         |
| 41         | YV           | 5          | VAL         |
| 41         | YV           | 10         | LYS         |
| 41         | YV           | 18         | LEU         |
| 41         | YV           | 19         | LYS         |
| 41         | YV           | 32         | THR         |
| 41         | YV           | 35         | LEU         |
| 41         | YV           | 47         | VAL         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | YV    | 64  | HIS  |
| 41  | YV    | 66  | ARG  |
| 41  | YV    | 73  | SER  |
| 41  | YV    | 78  | LYS  |
| 41  | YV    | 79  | VAL  |
| 41  | YV    | 80  | GLN  |
| 41  | YV    | 81  | TYR  |
| 41  | YV    | 82  | ARG  |
| 41  | YV    | 98  | GLU  |
| 41  | YV    | 100 | ARG  |
| 42  | YW    | 11  | ARG  |
| 42  | YW    | 17  | VAL  |
| 42  | YW    | 20  | VAL  |
| 42  | YW    | 50  | VAL  |
| 42  | YW    | 63  | ASP  |
| 42  | YW    | 66  | GLU  |
| 42  | YW    | 76  | VAL  |
| 42  | YW    | 88  | ARG  |
| 42  | YW    | 94  | ASP  |
| 42  | YW    | 96  | ILE  |
| 42  | YW    | 106 | ILE  |
| 42  | YW    | 107 | LEU  |
| 42  | YW    | 113 | LYS  |
| 43  | YX    | 27  | THR  |
| 43  | YX    | 48  | LYS  |
| 43  | YX    | 50  | LYS  |
| 43  | YX    | 53  | LYS  |
| 43  | YX    | 66  | LEU  |
| 43  | YX    | 80  | ILE  |
| 44  | YY    | 2   | ARG  |
| 44  | YY    | 5   | MET  |
| 44  | YY    | 9   | LYS  |
| 44  | YY    | 13  | VAL  |
| 44  | YY    | 14  | LEU  |
| 44  | YY    | 28  | LYS  |
| 44  | YY    | 33  | LYS  |
| 44  | YY    | 38  | ILE  |
| 44  | YY    | 40  | GLU  |
| 44  | YY    | 50  | ARG  |
| 44  | YY    | 51  | VAL  |
| 44  | YY    | 55  | TYR  |
| 44  | YY    | 60  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | YY    | 61  | ILE  |
| 44  | YY    | 62  | GLU  |
| 44  | YY    | 71  | LYS  |
| 44  | YY    | 75  | ILE  |
| 44  | YY    | 76  | CYS  |
| 44  | YY    | 86  | ARG  |
| 44  | YY    | 87  | LYS  |
| 44  | YY    | 95  | LYS  |
| 44  | YY    | 96  | ILE  |
| 44  | YY    | 97  | ARG  |
| 44  | YY    | 101 | LYS  |
| 45  | YZ    | 4   | ARG  |
| 45  | YZ    | 9   | TYR  |
| 45  | YZ    | 19  | ARG  |
| 45  | YZ    | 28  | MET  |
| 45  | YZ    | 33  | LEU  |
| 45  | YZ    | 34  | ASN  |
| 45  | YZ    | 41  | LEU  |
| 45  | YZ    | 61  | LEU  |
| 45  | YZ    | 71  | VAL  |
| 45  | YZ    | 75  | ASN  |
| 45  | YZ    | 76  | LEU  |
| 45  | YZ    | 81  | ARG  |
| 45  | YZ    | 87  | ASP  |
| 45  | YZ    | 91  | LEU  |
| 45  | YZ    | 104 | PHE  |
| 45  | YZ    | 107 | THR  |
| 45  | YZ    | 111 | VAL  |
| 45  | YZ    | 116 | VAL  |
| 45  | YZ    | 120 | ILE  |
| 45  | YZ    | 121 | HIS  |
| 45  | YZ    | 122 | ARG  |
| 45  | YZ    | 128 | VAL  |
| 45  | YZ    | 135 | GLU  |
| 45  | YZ    | 141 | VAL  |
| 45  | YZ    | 148 | ASP  |
| 45  | YZ    | 150 | LEU  |
| 45  | YZ    | 162 | GLU  |
| 45  | YZ    | 171 | ILE  |
| 46  | Y0    | 5   | LYS  |
| 46  | Y0    | 7   | LEU  |
| 46  | Y0    | 9   | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | Y0    | 10  | THR  |
| 46  | Y0    | 20  | ARG  |
| 46  | Y0    | 36  | ILE  |
| 46  | Y0    | 49  | LYS  |
| 46  | Y0    | 55  | ARG  |
| 47  | Y1    | 4   | VAL  |
| 47  | Y1    | 21  | ARG  |
| 47  | Y1    | 30  | VAL  |
| 47  | Y1    | 46  | LEU  |
| 47  | Y1    | 51  | VAL  |
| 47  | Y1    | 75  | GLU  |
| 47  | Y1    | 78  | LYS  |
| 47  | Y1    | 92  | LYS  |
| 47  | Y1    | 97  | LEU  |
| 47  | Y1    | 98  | LEU  |
| 48  | Y2    | 24  | LEU  |
| 48  | Y2    | 44  | LEU  |
| 48  | Y2    | 48  | HIS  |
| 48  | Y2    | 50  | ILE  |
| 48  | Y2    | 53  | LEU  |
| 48  | Y2    | 64  | LEU  |
| 48  | Y2    | 67  | LYS  |
| 49  | Y3    | 8   | LEU  |
| 49  | Y3    | 32  | GLN  |
| 49  | Y3    | 40  | THR  |
| 49  | Y3    | 54  | VAL  |
| 50  | Y4    | 6   | HIS  |
| 50  | Y4    | 16  | CYS  |
| 50  | Y4    | 18  | CYS  |
| 50  | Y4    | 21  | VAL  |
| 50  | Y4    | 31  | ILE  |
| 50  | Y4    | 34  | GLU  |
| 50  | Y4    | 35  | VAL  |
| 50  | Y4    | 36  | CYS  |
| 50  | Y4    | 37  | SER  |
| 50  | Y4    | 43  | TYR  |
| 50  | Y4    | 50  | VAL  |
| 50  | Y4    | 51  | ASP  |
| 50  | Y4    | 55  | ARG  |
| 50  | Y4    | 59  | PHE  |
| 50  | Y4    | 61  | ARG  |
| 50  | Y4    | 63  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | Y4    | 67  | TYR  |
| 50  | Y4    | 69  | LYS  |
| 51  | Y5    | 3   | LYS  |
| 51  | Y5    | 11  | THR  |
| 51  | Y5    | 23  | HIS  |
| 51  | Y5    | 26  | THR  |
| 51  | Y5    | 29  | THR  |
| 51  | Y5    | 52  | TYR  |
| 52  | Y6    | 7   | ILE  |
| 52  | Y6    | 8   | LYS  |
| 52  | Y6    | 9   | LEU  |
| 52  | Y6    | 10  | LEU  |
| 52  | Y6    | 12  | GLU  |
| 52  | Y6    | 18  | ARG  |
| 52  | Y6    | 21  | TYR  |
| 52  | Y6    | 24  | GLU  |
| 52  | Y6    | 28  | ARG  |
| 52  | Y6    | 34  | LEU  |
| 52  | Y6    | 37  | ARG  |
| 52  | Y6    | 38  | LYS  |
| 52  | Y6    | 39  | TYR  |
| 52  | Y6    | 40  | CYS  |
| 52  | Y6    | 44  | ARG  |
| 52  | Y6    | 45  | LYS  |
| 52  | Y6    | 47  | THR  |
| 53  | Y7    | 24  | THR  |
| 53  | Y7    | 33  | ARG  |
| 53  | Y7    | 43  | THR  |
| 53  | Y7    | 46  | VAL  |
| 53  | Y7    | 47  | ARG  |
| 53  | Y7    | 48  | LYS  |
| 53  | Y7    | 49  | ARG  |
| 54  | Y8    | 14  | VAL  |
| 54  | Y8    | 31  | HIS  |
| 54  | Y8    | 32  | LEU  |
| 54  | Y8    | 34  | TRP  |
| 54  | Y8    | 36  | LYS  |
| 54  | Y8    | 41  | ILE  |
| 54  | Y8    | 54  | GLU  |
| 54  | Y8    | 58  | ILE  |
| 54  | Y8    | 61  | LEU  |
| 54  | Y8    | 64  | TYR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | QC    | 63  | ASN  |
| 3   | QC    | 108 | ASN  |
| 7   | QG    | 86  | GLN  |
| 28  | RE    | 48  | GLN  |
| 28  | RE    | 55  | ASN  |
| 28  | RE    | 66  | HIS  |
| 40  | RU    | 81  | HIS  |
| 45  | RZ    | 118 | GLN  |
| 3   | XC    | 3   | ASN  |
| 3   | XC    | 108 | ASN  |
| 7   | XG    | 97  | GLN  |
| 9   | XI    | 117 | HIS  |
| 37  | YR    | 3   | HIS  |
| 50  | Y4    | 6   | HIS  |
| 50  | Y4    | 60  | GLN  |
| 52  | Y6    | 32  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | QA    | 1509/1522 (99%) | 295 (19%)         | 46 (3%)         |
| 1   | XA    | 1506/1522 (98%) | 290 (19%)         | 38 (2%)         |
| 22  | QV    | 76/77 (98%)     | 13 (17%)          | 0               |
| 22  | QW    | 76/77 (98%)     | 20 (26%)          | 2 (2%)          |
| 22  | XV    | 76/77 (98%)     | 12 (15%)          | 1 (1%)          |
| 22  | XW    | 76/77 (98%)     | 18 (23%)          | 0               |
| 23  | QX    | 19/25 (76%)     | 8 (42%)           | 2 (10%)         |
| 23  | XX    | 19/25 (76%)     | 9 (47%)           | 1 (5%)          |
| 25  | RA    | 2888/2916 (99%) | 590 (20%)         | 42 (1%)         |
| 25  | YA    | 2872/2916 (98%) | 567 (19%)         | 41 (1%)         |
| 26  | RB    | 121/124 (97%)   | 20 (16%)          | 1 (0%)          |
| 26  | YB    | 121/124 (97%)   | 21 (17%)          | 1 (0%)          |
| All | All   | 9359/9482 (98%) | 1863 (19%)        | 175 (1%)        |

All (1863) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 4   | U    |
| 1   | QA    | 5   | U    |
| 1   | QA    | 6   | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | QA    | 9      | G    |
| 1   | QA    | 22     | G    |
| 1   | QA    | 32     | A    |
| 1   | QA    | 39     | G    |
| 1   | QA    | 47     | C    |
| 1   | QA    | 48     | C    |
| 1   | QA    | 50     | A    |
| 1   | QA    | 51     | A    |
| 1   | QA    | 61     | G    |
| 1   | QA    | 64     | G    |
| 1   | QA    | 65     | U    |
| 1   | QA    | 66     | G    |
| 1   | QA    | 78     | G    |
| 1   | QA    | 79     | G    |
| 1   | QA    | 91     | C    |
| 1   | QA    | 93     | G    |
| 1   | QA    | 96     | U    |
| 1   | QA    | 101    | A    |
| 1   | QA    | 116    | A    |
| 1   | QA    | 121    | C    |
| 1   | QA    | 131    | C    |
| 1   | QA    | 163    | C    |
| 1   | QA    | 182    | U    |
| 1   | QA    | 186    | C    |
| 1   | QA    | 189(E) | U    |
| 1   | QA    | 189(F) | U    |
| 1   | QA    | 189(G) | G    |
| 1   | QA    | 189(H) | G    |
| 1   | QA    | 189(K) | U    |
| 1   | QA    | 189(L) | G    |
| 1   | QA    | 195    | A    |
| 1   | QA    | 197    | A    |
| 1   | QA    | 198    | G    |
| 1   | QA    | 201    | C    |
| 1   | QA    | 202    | U    |
| 1   | QA    | 203    | U    |
| 1   | QA    | 204    | U    |
| 1   | QA    | 216    | G    |
| 1   | QA    | 217    | C    |
| 1   | QA    | 244    | U    |
| 1   | QA    | 247    | G    |
| 1   | QA    | 251    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 266 | G    |
| 1   | QA    | 267 | C    |
| 1   | QA    | 280 | C    |
| 1   | QA    | 281 | G    |
| 1   | QA    | 289 | G    |
| 1   | QA    | 321 | A    |
| 1   | QA    | 328 | C    |
| 1   | QA    | 329 | A    |
| 1   | QA    | 332 | G    |
| 1   | QA    | 345 | C    |
| 1   | QA    | 346 | G    |
| 1   | QA    | 347 | G    |
| 1   | QA    | 350 | G    |
| 1   | QA    | 351 | G    |
| 1   | QA    | 352 | C    |
| 1   | QA    | 353 | A    |
| 1   | QA    | 354 | G    |
| 1   | QA    | 356 | A    |
| 1   | QA    | 367 | U    |
| 1   | QA    | 372 | C    |
| 1   | QA    | 373 | A    |
| 1   | QA    | 384 | G    |
| 1   | QA    | 397 | A    |
| 1   | QA    | 398 | C    |
| 1   | QA    | 406 | G    |
| 1   | QA    | 411 | A    |
| 1   | QA    | 412 | A    |
| 1   | QA    | 422 | C    |
| 1   | QA    | 423 | G    |
| 1   | QA    | 429 | U    |
| 1   | QA    | 430 | A    |
| 1   | QA    | 439 | A    |
| 1   | QA    | 442 | C    |
| 1   | QA    | 470 | C    |
| 1   | QA    | 474 | G    |
| 1   | QA    | 477 | A    |
| 1   | QA    | 482 | A    |
| 1   | QA    | 485 | G    |
| 1   | QA    | 486 | U    |
| 1   | QA    | 494 | U    |
| 1   | QA    | 495 | A    |
| 1   | QA    | 498 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 505 | G    |
| 1   | QA    | 511 | C    |
| 1   | QA    | 518 | C    |
| 1   | QA    | 519 | C    |
| 1   | QA    | 521 | G    |
| 1   | QA    | 527 | G    |
| 1   | QA    | 532 | A    |
| 1   | QA    | 533 | A    |
| 1   | QA    | 545 | C    |
| 1   | QA    | 547 | A    |
| 1   | QA    | 548 | G    |
| 1   | QA    | 559 | A    |
| 1   | QA    | 561 | U    |
| 1   | QA    | 572 | A    |
| 1   | QA    | 573 | A    |
| 1   | QA    | 576 | G    |
| 1   | QA    | 577 | G    |
| 1   | QA    | 579 | G    |
| 1   | QA    | 594 | G    |
| 1   | QA    | 595 | G    |
| 1   | QA    | 596 | C    |
| 1   | QA    | 617 | G    |
| 1   | QA    | 630 | G    |
| 1   | QA    | 653 | A    |
| 1   | QA    | 665 | A    |
| 1   | QA    | 688 | G    |
| 1   | QA    | 701 | C    |
| 1   | QA    | 702 | A    |
| 1   | QA    | 703 | G    |
| 1   | QA    | 704 | A    |
| 1   | QA    | 717 | C    |
| 1   | QA    | 721 | G    |
| 1   | QA    | 722 | A    |
| 1   | QA    | 724 | G    |
| 1   | QA    | 731 | G    |
| 1   | QA    | 749 | C    |
| 1   | QA    | 755 | G    |
| 1   | QA    | 760 | G    |
| 1   | QA    | 777 | A    |
| 1   | QA    | 786 | G    |
| 1   | QA    | 792 | A    |
| 1   | QA    | 793 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | QA    | 794     | A    |
| 1   | QA    | 813     | U    |
| 1   | QA    | 815     | A    |
| 1   | QA    | 817     | C    |
| 1   | QA    | 821     | G    |
| 1   | QA    | 828     | A    |
| 1   | QA    | 839     | U    |
| 1   | QA    | 840     | C    |
| 1   | QA    | 841     | U    |
| 1   | QA    | 848     | C    |
| 1   | QA    | 859     | A    |
| 1   | QA    | 870     | U    |
| 1   | QA    | 871     | U    |
| 1   | QA    | 872     | A    |
| 1   | QA    | 874     | G    |
| 1   | QA    | 914     | A    |
| 1   | QA    | 926     | G    |
| 1   | QA    | 927     | G    |
| 1   | QA    | 934     | C    |
| 1   | QA    | 935     | A    |
| 1   | QA    | 960     | U    |
| 1   | QA    | 961     | U    |
| 1   | QA    | 966     | G    |
| 1   | QA    | 969     | A    |
| 1   | QA    | 971     | G    |
| 1   | QA    | 974     | A    |
| 1   | QA    | 977     | A    |
| 1   | QA    | 978     | A    |
| 1   | QA    | 980     | C    |
| 1   | QA    | 991     | U    |
| 1   | QA    | 992     | U    |
| 1   | QA    | 993     | G    |
| 1   | QA    | 1000    | U    |
| 1   | QA    | 1001    | A    |
| 1   | QA    | 1001(A) | G    |
| 1   | QA    | 1003    | G    |
| 1   | QA    | 1005    | A    |
| 1   | QA    | 1006    | C    |
| 1   | QA    | 1007    | C    |
| 1   | QA    | 1008    | C    |
| 1   | QA    | 1009    | G    |
| 1   | QA    | 1020    | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | QA    | 1021    | G    |
| 1   | QA    | 1024    | G    |
| 1   | QA    | 1025    | U    |
| 1   | QA    | 1026    | G    |
| 1   | QA    | 1030(A) | G    |
| 1   | QA    | 1030(C) | G    |
| 1   | QA    | 1030(D) | A    |
| 1   | QA    | 1031    | G    |
| 1   | QA    | 1033    | G    |
| 1   | QA    | 1034    | G    |
| 1   | QA    | 1036    | G    |
| 1   | QA    | 1038    | C    |
| 1   | QA    | 1039    | C    |
| 1   | QA    | 1042    | G    |
| 1   | QA    | 1053    | G    |
| 1   | QA    | 1054    | C    |
| 1   | QA    | 1064    | G    |
| 1   | QA    | 1065    | U    |
| 1   | QA    | 1066    | C    |
| 1   | QA    | 1067    | A    |
| 1   | QA    | 1068    | G    |
| 1   | QA    | 1081    | G    |
| 1   | QA    | 1086    | U    |
| 1   | QA    | 1094    | G    |
| 1   | QA    | 1095    | U    |
| 1   | QA    | 1101    | A    |
| 1   | QA    | 1118    | C    |
| 1   | QA    | 1124    | G    |
| 1   | QA    | 1125    | U    |
| 1   | QA    | 1136    | U    |
| 1   | QA    | 1137    | C    |
| 1   | QA    | 1138    | G    |
| 1   | QA    | 1139    | G    |
| 1   | QA    | 1140    | C    |
| 1   | QA    | 1146    | A    |
| 1   | QA    | 1152    | A    |
| 1   | QA    | 1157    | A    |
| 1   | QA    | 1158    | C    |
| 1   | QA    | 1159    | U    |
| 1   | QA    | 1160    | G    |
| 1   | QA    | 1176    | A    |
| 1   | QA    | 1177    | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | QA           | 1178       | G           |
| 1          | QA           | 1181       | G           |
| 1          | QA           | 1183       | A           |
| 1          | QA           | 1190       | G           |
| 1          | QA           | 1193       | G           |
| 1          | QA           | 1196       | U           |
| 1          | QA           | 1197       | G           |
| 1          | QA           | 1212       | U           |
| 1          | QA           | 1213       | A           |
| 1          | QA           | 1225       | A           |
| 1          | QA           | 1226       | C           |
| 1          | QA           | 1237       | C           |
| 1          | QA           | 1238       | A           |
| 1          | QA           | 1240       | U           |
| 1          | QA           | 1241       | G           |
| 1          | QA           | 1256       | A           |
| 1          | QA           | 1257       | U           |
| 1          | QA           | 1258       | G           |
| 1          | QA           | 1273       | G           |
| 1          | QA           | 1278       | U           |
| 1          | QA           | 1280       | A           |
| 1          | QA           | 1281       | U           |
| 1          | QA           | 1285       | A           |
| 1          | QA           | 1286       | A           |
| 1          | QA           | 1287       | A           |
| 1          | QA           | 1288       | A           |
| 1          | QA           | 1297       | C           |
| 1          | QA           | 1298       | C           |
| 1          | QA           | 1299       | A           |
| 1          | QA           | 1301       | U           |
| 1          | QA           | 1302       | U           |
| 1          | QA           | 1303       | C           |
| 1          | QA           | 1305       | G           |
| 1          | QA           | 1312       | G           |
| 1          | QA           | 1320       | C           |
| 1          | QA           | 1322       | C           |
| 1          | QA           | 1323       | G           |
| 1          | QA           | 1331       | G           |
| 1          | QA           | 1335       | C           |
| 1          | QA           | 1337       | G           |
| 1          | QA           | 1338       | G           |
| 1          | QA           | 1346       | A           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | QA    | 1347    | G    |
| 1   | QA    | 1348    | U    |
| 1   | QA    | 1353    | G    |
| 1   | QA    | 1363    | C    |
| 1   | QA    | 1364    | U    |
| 1   | QA    | 1370    | G    |
| 1   | QA    | 1379    | G    |
| 1   | QA    | 1382    | C    |
| 1   | QA    | 1397    | C    |
| 1   | QA    | 1398    | A    |
| 1   | QA    | 1406    | U    |
| 1   | QA    | 1419    | G    |
| 1   | QA    | 1442    | G    |
| 1   | QA    | 1442(B) | A    |
| 1   | QA    | 1446    | U    |
| 1   | QA    | 1447    | A    |
| 1   | QA    | 1452    | C    |
| 1   | QA    | 1456    | G    |
| 1   | QA    | 1457    | G    |
| 1   | QA    | 1475    | G    |
| 1   | QA    | 1491    | G    |
| 1   | QA    | 1493    | A    |
| 1   | QA    | 1497    | G    |
| 1   | QA    | 1499    | A    |
| 1   | QA    | 1502    | A    |
| 1   | QA    | 1504    | G    |
| 1   | QA    | 1505    | G    |
| 1   | QA    | 1506    | U    |
| 1   | QA    | 1517    | G    |
| 1   | QA    | 1519    | A    |
| 1   | QA    | 1520    | G    |
| 1   | QA    | 1529    | G    |
| 1   | QA    | 1530    | G    |
| 1   | QA    | 1532    | U    |
| 1   | QA    | 1533    | C    |
| 1   | QA    | 1534    | A    |
| 1   | QA    | 1536    | C    |
| 1   | QA    | 1540    | U    |
| 1   | QA    | 1541    | U    |
| 1   | QA    | 1542    | U    |
| 22  | QV    | 3       | C    |
| 22  | QV    | 8       | U    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 22  | QV    | 14    | A    |
| 22  | QV    | 17(A) | U    |
| 22  | QV    | 18    | G    |
| 22  | QV    | 19    | G    |
| 22  | QV    | 20    | U    |
| 22  | QV    | 21    | A    |
| 22  | QV    | 47    | U    |
| 22  | QV    | 48    | C    |
| 22  | QV    | 49    | G    |
| 22  | QV    | 65    | C    |
| 22  | QV    | 76    | A    |
| 22  | QW    | 8     | U    |
| 22  | QW    | 10    | G    |
| 22  | QW    | 14    | A    |
| 22  | QW    | 15    | G    |
| 22  | QW    | 16    | C    |
| 22  | QW    | 17    | C    |
| 22  | QW    | 17(A) | U    |
| 22  | QW    | 18    | G    |
| 22  | QW    | 20    | U    |
| 22  | QW    | 21    | A    |
| 22  | QW    | 22    | G    |
| 22  | QW    | 34    | C    |
| 22  | QW    | 47    | U    |
| 22  | QW    | 48    | C    |
| 22  | QW    | 49    | G    |
| 22  | QW    | 50    | U    |
| 22  | QW    | 55    | U    |
| 22  | QW    | 56    | C    |
| 22  | QW    | 61    | C    |
| 22  | QW    | 72    | A    |
| 23  | QX    | 10    | G    |
| 23  | QX    | 12    | A    |
| 23  | QX    | 13    | A    |
| 23  | QX    | 14    | A    |
| 23  | QX    | 17    | U    |
| 23  | QX    | 19    | A2M  |
| 23  | QX    | 20    | A2M  |
| 23  | QX    | 21    | A2M  |
| 25  | RA    | 9     | U    |
| 25  | RA    | 15    | G    |
| 25  | RA    | 28    | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 34         | C           |
| 25         | RA           | 35         | G           |
| 25         | RA           | 45         | C           |
| 25         | RA           | 49         | A           |
| 25         | RA           | 51         | G           |
| 25         | RA           | 58         | G           |
| 25         | RA           | 60         | G           |
| 25         | RA           | 69         | C           |
| 25         | RA           | 71         | A           |
| 25         | RA           | 75         | G           |
| 25         | RA           | 82         | G           |
| 25         | RA           | 90         | U           |
| 25         | RA           | 92         | A           |
| 25         | RA           | 94         | C           |
| 25         | RA           | 95         | G           |
| 25         | RA           | 100        | G           |
| 25         | RA           | 102        | G           |
| 25         | RA           | 113        | G           |
| 25         | RA           | 118        | A           |
| 25         | RA           | 120        | U           |
| 25         | RA           | 129        | C           |
| 25         | RA           | 137        | C           |
| 25         | RA           | 139(A)     | G           |
| 25         | RA           | 140        | G           |
| 25         | RA           | 141        | A           |
| 25         | RA           | 142        | A           |
| 25         | RA           | 154        | G           |
| 25         | RA           | 154(A)     | C           |
| 25         | RA           | 174        | C           |
| 25         | RA           | 175        | G           |
| 25         | RA           | 181        | A           |
| 25         | RA           | 196        | A           |
| 25         | RA           | 199        | A           |
| 25         | RA           | 215        | G           |
| 25         | RA           | 216        | A           |
| 25         | RA           | 221        | A           |
| 25         | RA           | 222        | A           |
| 25         | RA           | 225        | A           |
| 25         | RA           | 228        | A           |
| 25         | RA           | 229        | A           |
| 25         | RA           | 248        | G           |
| 25         | RA           | 249        | C           |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | RA    | 252    | G    |
| 25  | RA    | 260    | G    |
| 25  | RA    | 261    | G    |
| 25  | RA    | 267    | C    |
| 25  | RA    | 268    | C    |
| 25  | RA    | 269    | U    |
| 25  | RA    | 271(J) | C    |
| 25  | RA    | 271(K) | U    |
| 25  | RA    | 271(L) | U    |
| 25  | RA    | 271(N) | U    |
| 25  | RA    | 271(O) | C    |
| 25  | RA    | 271(P) | C    |
| 25  | RA    | 271(Y) | U    |
| 25  | RA    | 272(A) | U    |
| 25  | RA    | 272(B) | G    |
| 25  | RA    | 272(H) | C    |
| 25  | RA    | 274    | G    |
| 25  | RA    | 278    | A    |
| 25  | RA    | 283    | A    |
| 25  | RA    | 284    | U    |
| 25  | RA    | 288    | C    |
| 25  | RA    | 289    | A    |
| 25  | RA    | 311    | A    |
| 25  | RA    | 324    | A    |
| 25  | RA    | 329    | G    |
| 25  | RA    | 330    | A    |
| 25  | RA    | 332    | A    |
| 25  | RA    | 345    | A    |
| 25  | RA    | 352    | G    |
| 25  | RA    | 353    | G    |
| 25  | RA    | 356    | G    |
| 25  | RA    | 358    | U    |
| 25  | RA    | 362    | U    |
| 25  | RA    | 363    | G    |
| 25  | RA    | 363(E) | U    |
| 25  | RA    | 363(F) | A    |
| 25  | RA    | 364    | C    |
| 25  | RA    | 371    | A    |
| 25  | RA    | 372    | G    |
| 25  | RA    | 373    | U    |
| 25  | RA    | 374    | A    |
| 25  | RA    | 386    | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 388        | G           |
| 25         | RA           | 396        | G           |
| 25         | RA           | 405        | U           |
| 25         | RA           | 407        | G           |
| 25         | RA           | 411        | G           |
| 25         | RA           | 412        | A           |
| 25         | RA           | 428        | A           |
| 25         | RA           | 443        | A           |
| 25         | RA           | 444        | C           |
| 25         | RA           | 448        | U           |
| 25         | RA           | 455        | C           |
| 25         | RA           | 457        | A           |
| 25         | RA           | 470        | A           |
| 25         | RA           | 481        | G           |
| 25         | RA           | 494        | G           |
| 25         | RA           | 505        | A           |
| 25         | RA           | 509        | C           |
| 25         | RA           | 512        | G           |
| 25         | RA           | 528        | A           |
| 25         | RA           | 530        | G           |
| 25         | RA           | 531        | C           |
| 25         | RA           | 532        | A           |
| 25         | RA           | 533        | G           |
| 25         | RA           | 544        | G           |
| 25         | RA           | 549        | G           |
| 25         | RA           | 556        | G           |
| 25         | RA           | 561        | G           |
| 25         | RA           | 562        | U           |
| 25         | RA           | 563        | G           |
| 25         | RA           | 573        | G           |
| 25         | RA           | 574        | C           |
| 25         | RA           | 575        | A           |
| 25         | RA           | 586        | A           |
| 25         | RA           | 587        | C           |
| 25         | RA           | 588        | U           |
| 25         | RA           | 593        | G           |
| 25         | RA           | 603        | A           |
| 25         | RA           | 604        | G           |
| 25         | RA           | 607        | U           |
| 25         | RA           | 614        | U           |
| 25         | RA           | 614(A)     | U           |
| 25         | RA           | 614(B)     | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 615        | G           |
| 25         | RA           | 627        | A           |
| 25         | RA           | 637        | A           |
| 25         | RA           | 645        | C           |
| 25         | RA           | 646        | A           |
| 25         | RA           | 651        | G           |
| 25         | RA           | 654        | A           |
| 25         | RA           | 654(A)     | G           |
| 25         | RA           | 654(B)     | C           |
| 25         | RA           | 654(F)     | C           |
| 25         | RA           | 654(G)     | C           |
| 25         | RA           | 654(O)     | G           |
| 25         | RA           | 654(Q)     | C           |
| 25         | RA           | 654(R)     | C           |
| 25         | RA           | 654(S)     | G           |
| 25         | RA           | 654(T)     | C           |
| 25         | RA           | 657        | U           |
| 25         | RA           | 668        | G           |
| 25         | RA           | 686        | G           |
| 25         | RA           | 708        | C           |
| 25         | RA           | 717        | G           |
| 25         | RA           | 722        | A           |
| 25         | RA           | 726        | G           |
| 25         | RA           | 730        | C           |
| 25         | RA           | 739        | G           |
| 25         | RA           | 740        | U           |
| 25         | RA           | 748        | G           |
| 25         | RA           | 749        | C           |
| 25         | RA           | 753        | C           |
| 25         | RA           | 782        | A           |
| 25         | RA           | 784        | A           |
| 25         | RA           | 785        | G           |
| 25         | RA           | 789        | A           |
| 25         | RA           | 792        | G           |
| 25         | RA           | 805        | G           |
| 25         | RA           | 812        | C           |
| 25         | RA           | 819        | A           |
| 25         | RA           | 827        | U           |
| 25         | RA           | 828        | U           |
| 25         | RA           | 845        | G           |
| 25         | RA           | 855        | G           |
| 25         | RA           | 856        | C           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | RA    | 857  | C    |
| 25  | RA    | 859  | G    |
| 25  | RA    | 860  | U    |
| 25  | RA    | 862  | G    |
| 25  | RA    | 865  | C    |
| 25  | RA    | 866  | A    |
| 25  | RA    | 878  | A    |
| 25  | RA    | 879  | G    |
| 25  | RA    | 881  | G    |
| 25  | RA    | 882  | G    |
| 25  | RA    | 883  | G    |
| 25  | RA    | 884  | C    |
| 25  | RA    | 888  | C    |
| 25  | RA    | 889  | C    |
| 25  | RA    | 890  | A    |
| 25  | RA    | 894  | C    |
| 25  | RA    | 895  | U    |
| 25  | RA    | 896  | A    |
| 25  | RA    | 897  | C    |
| 25  | RA    | 901  | A    |
| 25  | RA    | 910  | A    |
| 25  | RA    | 917  | A    |
| 25  | RA    | 927  | G    |
| 25  | RA    | 932  | G    |
| 25  | RA    | 934  | G    |
| 25  | RA    | 941  | A    |
| 25  | RA    | 945  | A    |
| 25  | RA    | 946  | G    |
| 25  | RA    | 953  | A    |
| 25  | RA    | 961  | C    |
| 25  | RA    | 974  | G    |
| 25  | RA    | 983  | A    |
| 25  | RA    | 989  | G    |
| 25  | RA    | 990  | A    |
| 25  | RA    | 991  | C    |
| 25  | RA    | 996  | A    |
| 25  | RA    | 1010 | A    |
| 25  | RA    | 1011 | G    |
| 25  | RA    | 1012 | U    |
| 25  | RA    | 1013 | C    |
| 25  | RA    | 1017 | G    |
| 25  | RA    | 1022 | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 1023       | U           |
| 25         | RA           | 1025       | G           |
| 25         | RA           | 1026       | U           |
| 25         | RA           | 1027       | A           |
| 25         | RA           | 1033       | U           |
| 25         | RA           | 1034       | G           |
| 25         | RA           | 1036       | G           |
| 25         | RA           | 1044       | G           |
| 25         | RA           | 1045       | A           |
| 25         | RA           | 1046       | A           |
| 25         | RA           | 1047       | G           |
| 25         | RA           | 1049       | C           |
| 25         | RA           | 1060       | U           |
| 25         | RA           | 1061       | U           |
| 25         | RA           | 1070       | A           |
| 25         | RA           | 1086       | A           |
| 25         | RA           | 1087       | G           |
| 25         | RA           | 1088       | A           |
| 25         | RA           | 1089       | G           |
| 25         | RA           | 1095       | A           |
| 25         | RA           | 1096       | A           |
| 25         | RA           | 1099       | G           |
| 25         | RA           | 1122       | G           |
| 25         | RA           | 1130       | U           |
| 25         | RA           | 1135       | C           |
| 25         | RA           | 1136       | G           |
| 25         | RA           | 1139       | G           |
| 25         | RA           | 1142       | U           |
| 25         | RA           | 1142(A)    | A           |
| 25         | RA           | 1155       | A           |
| 25         | RA           | 1167       | U           |
| 25         | RA           | 1173       | G           |
| 25         | RA           | 1174       | A           |
| 25         | RA           | 1175       | U           |
| 25         | RA           | 1176       | G           |
| 25         | RA           | 1177       | A           |
| 25         | RA           | 1178       | C           |
| 25         | RA           | 1180       | C           |
| 25         | RA           | 1195       | G           |
| 25         | RA           | 1220       | A           |
| 25         | RA           | 1236       | G           |
| 25         | RA           | 1249       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 1250       | G           |
| 25         | RA           | 1253       | A           |
| 25         | RA           | 1254       | A           |
| 25         | RA           | 1255       | U           |
| 25         | RA           | 1256       | G           |
| 25         | RA           | 1265       | A           |
| 25         | RA           | 1271       | G           |
| 25         | RA           | 1272       | A           |
| 25         | RA           | 1281       | G           |
| 25         | RA           | 1286       | A           |
| 25         | RA           | 1289       | C           |
| 25         | RA           | 1300       | U           |
| 25         | RA           | 1301       | A           |
| 25         | RA           | 1308       | A           |
| 25         | RA           | 1311       | G           |
| 25         | RA           | 1313       | U           |
| 25         | RA           | 1314       | C           |
| 25         | RA           | 1319       | G           |
| 25         | RA           | 1329       | U           |
| 25         | RA           | 1341       | U           |
| 25         | RA           | 1342       | A           |
| 25         | RA           | 1346       | G           |
| 25         | RA           | 1352       | U           |
| 25         | RA           | 1359       | A           |
| 25         | RA           | 1360       | A           |
| 25         | RA           | 1365       | A           |
| 25         | RA           | 1367       | A           |
| 25         | RA           | 1368       | G           |
| 25         | RA           | 1379       | A           |
| 25         | RA           | 1384       | A           |
| 25         | RA           | 1385       | G           |
| 25         | RA           | 1392       | A           |
| 25         | RA           | 1406       | U           |
| 25         | RA           | 1407       | C           |
| 25         | RA           | 1416       | G           |
| 25         | RA           | 1420       | U           |
| 25         | RA           | 1421       | G           |
| 25         | RA           | 1428       | C           |
| 25         | RA           | 1432       | C           |
| 25         | RA           | 1437       | C           |
| 25         | RA           | 1445       | A           |
| 25         | RA           | 1449       | A           |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | RA    | 1450    | G    |
| 25  | RA    | 1452    | A    |
| 25  | RA    | 1455    | G    |
| 25  | RA    | 1459    | G    |
| 25  | RA    | 1460    | A    |
| 25  | RA    | 1461    | G    |
| 25  | RA    | 1467    | C    |
| 25  | RA    | 1471    | A    |
| 25  | RA    | 1475    | G    |
| 25  | RA    | 1476    | C    |
| 25  | RA    | 1477    | A    |
| 25  | RA    | 1481    | U    |
| 25  | RA    | 1482    | G    |
| 25  | RA    | 1485    | G    |
| 25  | RA    | 1488    | G    |
| 25  | RA    | 1490    | A    |
| 25  | RA    | 1493    | C    |
| 25  | RA    | 1505    | C    |
| 25  | RA    | 1509    | C    |
| 25  | RA    | 1509(A) | A    |
| 25  | RA    | 1520    | G    |
| 25  | RA    | 1534    | G    |
| 25  | RA    | 1535    | U    |
| 25  | RA    | 1536    | A    |
| 25  | RA    | 1537    | C    |
| 25  | RA    | 1538    | G    |
| 25  | RA    | 1543    | A    |
| 25  | RA    | 1545    | A    |
| 25  | RA    | 1547    | C    |
| 25  | RA    | 1550    | C    |
| 25  | RA    | 1554    | A    |
| 25  | RA    | 1558    | A    |
| 25  | RA    | 1566    | A    |
| 25  | RA    | 1569    | A    |
| 25  | RA    | 1578    | U    |
| 25  | RA    | 1581    | G    |
| 25  | RA    | 1584    | C    |
| 25  | RA    | 1586    | A    |
| 25  | RA    | 1588    | C    |
| 25  | RA    | 1598    | C    |
| 25  | RA    | 1608    | A    |
| 25  | RA    | 1640    | C    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 1648       | C           |
| 25         | RA           | 1654       | A           |
| 25         | RA           | 1674       | G           |
| 25         | RA           | 1681       | G           |
| 25         | RA           | 1695       | G           |
| 25         | RA           | 1696       | G           |
| 25         | RA           | 1700       | A           |
| 25         | RA           | 1701       | A           |
| 25         | RA           | 1717       | G           |
| 25         | RA           | 1718       | G           |
| 25         | RA           | 1721       | G           |
| 25         | RA           | 1722       | A           |
| 25         | RA           | 1740       | G           |
| 25         | RA           | 1744       | C           |
| 25         | RA           | 1746       | G           |
| 25         | RA           | 1756       | G           |
| 25         | RA           | 1763       | G           |
| 25         | RA           | 1764       | G           |
| 25         | RA           | 1773       | A           |
| 25         | RA           | 1780       | A           |
| 25         | RA           | 1791       | A           |
| 25         | RA           | 1800       | C           |
| 25         | RA           | 1801       | G           |
| 25         | RA           | 1816       | G           |
| 25         | RA           | 1820       | U           |
| 25         | RA           | 1829       | A           |
| 25         | RA           | 1835       | G           |
| 25         | RA           | 1839       | G           |
| 25         | RA           | 1847       | A           |
| 25         | RA           | 1860       | G           |
| 25         | RA           | 1865       | G           |
| 25         | RA           | 1877       | A           |
| 25         | RA           | 1878       | G           |
| 25         | RA           | 1880       | C           |
| 25         | RA           | 1882       | C           |
| 25         | RA           | 1889       | A           |
| 25         | RA           | 1900       | A           |
| 25         | RA           | 1903       | G           |
| 25         | RA           | 1906       | G           |
| 25         | RA           | 1913       | A           |
| 25         | RA           | 1914       | C           |
| 25         | RA           | 1916       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 1929       | G           |
| 25         | RA           | 1930       | G           |
| 25         | RA           | 1931       | U           |
| 25         | RA           | 1936       | A           |
| 25         | RA           | 1938       | A           |
| 25         | RA           | 1948       | G           |
| 25         | RA           | 1949       | G           |
| 25         | RA           | 1955       | U           |
| 25         | RA           | 1963       | U           |
| 25         | RA           | 1967       | C           |
| 25         | RA           | 1970       | A           |
| 25         | RA           | 1971       | A           |
| 25         | RA           | 1972       | A           |
| 25         | RA           | 1980       | G           |
| 25         | RA           | 1982       | C           |
| 25         | RA           | 1992       | G           |
| 25         | RA           | 1993       | U           |
| 25         | RA           | 2020       | A           |
| 25         | RA           | 2022       | U           |
| 25         | RA           | 2023       | G           |
| 25         | RA           | 2027       | G           |
| 25         | RA           | 2031       | A           |
| 25         | RA           | 2032       | G           |
| 25         | RA           | 2033       | A           |
| 25         | RA           | 2043       | C           |
| 25         | RA           | 2052       | G           |
| 25         | RA           | 2055       | C           |
| 25         | RA           | 2056       | G           |
| 25         | RA           | 2059       | A           |
| 25         | RA           | 2060       | A           |
| 25         | RA           | 2061       | G           |
| 25         | RA           | 2062       | A           |
| 25         | RA           | 2063       | C           |
| 25         | RA           | 2069       | G           |
| 25         | RA           | 2092       | U           |
| 25         | RA           | 2093       | G           |
| 25         | RA           | 2096       | U           |
| 25         | RA           | 2099       | U           |
| 25         | RA           | 2108       | C           |
| 25         | RA           | 2111       | C           |
| 25         | RA           | 2112       | G           |
| 25         | RA           | 2113       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 2114       | A           |
| 25         | RA           | 2116       | G           |
| 25         | RA           | 2117       | A           |
| 25         | RA           | 2120       | G           |
| 25         | RA           | 2123       | G           |
| 25         | RA           | 2128       | C           |
| 25         | RA           | 2130       | U           |
| 25         | RA           | 2131       | G           |
| 25         | RA           | 2132       | U           |
| 25         | RA           | 2140       | C           |
| 25         | RA           | 2145       | C           |
| 25         | RA           | 2147       | G           |
| 25         | RA           | 2148       | G           |
| 25         | RA           | 2165       | G           |
| 25         | RA           | 2167       | U           |
| 25         | RA           | 2168       | G           |
| 25         | RA           | 2169       | A           |
| 25         | RA           | 2171       | A           |
| 25         | RA           | 2173       | A           |
| 25         | RA           | 2190       | G           |
| 25         | RA           | 2192       | G           |
| 25         | RA           | 2198       | A           |
| 25         | RA           | 2199       | A           |
| 25         | RA           | 2203       | U           |
| 25         | RA           | 2206       | G           |
| 25         | RA           | 2207       | G           |
| 25         | RA           | 2208       | A           |
| 25         | RA           | 2218       | U           |
| 25         | RA           | 2219       | G           |
| 25         | RA           | 2225       | A           |
| 25         | RA           | 2226       | C           |
| 25         | RA           | 2238       | G           |
| 25         | RA           | 2239       | G           |
| 25         | RA           | 2246       | G           |
| 25         | RA           | 2275       | C           |
| 25         | RA           | 2276       | G           |
| 25         | RA           | 2279       | G           |
| 25         | RA           | 2283       | C           |
| 25         | RA           | 2287       | A           |
| 25         | RA           | 2288       | A           |
| 25         | RA           | 2305       | A           |
| 25         | RA           | 2307       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 2308       | G           |
| 25         | RA           | 2309       | A           |
| 25         | RA           | 2312       | U           |
| 25         | RA           | 2316       | C           |
| 25         | RA           | 2320       | A           |
| 25         | RA           | 2325       | G           |
| 25         | RA           | 2334       | G           |
| 25         | RA           | 2335       | A           |
| 25         | RA           | 2336       | A           |
| 25         | RA           | 2343       | C           |
| 25         | RA           | 2345       | G           |
| 25         | RA           | 2347       | C           |
| 25         | RA           | 2350       | C           |
| 25         | RA           | 2382       | G           |
| 25         | RA           | 2383       | G           |
| 25         | RA           | 2385       | C           |
| 25         | RA           | 2394       | C           |
| 25         | RA           | 2402       | C           |
| 25         | RA           | 2406       | U           |
| 25         | RA           | 2410       | G           |
| 25         | RA           | 2414       | G           |
| 25         | RA           | 2422       | A           |
| 25         | RA           | 2423       | U           |
| 25         | RA           | 2424       | C           |
| 25         | RA           | 2425       | A           |
| 25         | RA           | 2429       | G           |
| 25         | RA           | 2430       | A           |
| 25         | RA           | 2435       | A           |
| 25         | RA           | 2439       | A           |
| 25         | RA           | 2440       | C           |
| 25         | RA           | 2441       | C           |
| 25         | RA           | 2445       | G           |
| 25         | RA           | 2447       | G           |
| 25         | RA           | 2448       | A           |
| 25         | RA           | 2468       | G           |
| 25         | RA           | 2469       | A           |
| 25         | RA           | 2470       | G           |
| 25         | RA           | 2471       | C           |
| 25         | RA           | 2472       | G           |
| 25         | RA           | 2474       | C           |
| 25         | RA           | 2475       | C           |
| 25         | RA           | 2476       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 2482       | G           |
| 25         | RA           | 2484       | G           |
| 25         | RA           | 2494       | G           |
| 25         | RA           | 2502       | G           |
| 25         | RA           | 2505       | G           |
| 25         | RA           | 2518       | A           |
| 25         | RA           | 2519       | U           |
| 25         | RA           | 2529       | G           |
| 25         | RA           | 2535       | G           |
| 25         | RA           | 2541       | A           |
| 25         | RA           | 2542       | A           |
| 25         | RA           | 2543       | G           |
| 25         | RA           | 2546       | U           |
| 25         | RA           | 2554       | U           |
| 25         | RA           | 2566       | A           |
| 25         | RA           | 2567       | G           |
| 25         | RA           | 2569       | G           |
| 25         | RA           | 2572       | A           |
| 25         | RA           | 2573       | C           |
| 25         | RA           | 2601       | C           |
| 25         | RA           | 2602       | A           |
| 25         | RA           | 2603       | G           |
| 25         | RA           | 2609       | U           |
| 25         | RA           | 2610       | C           |
| 25         | RA           | 2611       | U           |
| 25         | RA           | 2612       | C           |
| 25         | RA           | 2615       | U           |
| 25         | RA           | 2629       | A           |
| 25         | RA           | 2630       | G           |
| 25         | RA           | 2646       | C           |
| 25         | RA           | 2654       | A           |
| 25         | RA           | 2655       | G           |
| 25         | RA           | 2665       | A           |
| 25         | RA           | 2673       | G           |
| 25         | RA           | 2675       | A           |
| 25         | RA           | 2682       | U           |
| 25         | RA           | 2689       | U           |
| 25         | RA           | 2690       | C           |
| 25         | RA           | 2691       | C           |
| 25         | RA           | 2702       | U           |
| 25         | RA           | 2703       | C           |
| 25         | RA           | 2712       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | RA           | 2712(A)    | A           |
| 25         | RA           | 2713       | A           |
| 25         | RA           | 2714       | G           |
| 25         | RA           | 2726       | U           |
| 25         | RA           | 2732       | G           |
| 25         | RA           | 2733       | A           |
| 25         | RA           | 2744       | G           |
| 25         | RA           | 2748       | A           |
| 25         | RA           | 2758       | A           |
| 25         | RA           | 2762       | G           |
| 25         | RA           | 2765       | A           |
| 25         | RA           | 2766       | G           |
| 25         | RA           | 2770       | G           |
| 25         | RA           | 2777       | G           |
| 25         | RA           | 2778       | A           |
| 25         | RA           | 2790       | A           |
| 25         | RA           | 2791       | C           |
| 25         | RA           | 2792       | G           |
| 25         | RA           | 2807       | G           |
| 25         | RA           | 2808       | U           |
| 25         | RA           | 2818       | G           |
| 25         | RA           | 2820       | A           |
| 25         | RA           | 2821       | A           |
| 25         | RA           | 2823       | A           |
| 25         | RA           | 2827       | C           |
| 25         | RA           | 2833       | G           |
| 25         | RA           | 2834       | G           |
| 25         | RA           | 2845       | G           |
| 25         | RA           | 2849       | U           |
| 25         | RA           | 2850       | A           |
| 25         | RA           | 2860       | A           |
| 25         | RA           | 2867       | G           |
| 25         | RA           | 2868       | A           |
| 25         | RA           | 2872       | G           |
| 25         | RA           | 2876       | G           |
| 25         | RA           | 2877       | G           |
| 25         | RA           | 2879       | C           |
| 25         | RA           | 2880       | C           |
| 25         | RA           | 2893       | G           |
| 25         | RA           | 2894       | G           |
| 25         | RA           | 2896       | C           |
| 26         | RB           | 0          | A           |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | RB    | 8   | U    |
| 26  | RB    | 13  | A    |
| 26  | RB    | 14  | U    |
| 26  | RB    | 15  | A    |
| 26  | RB    | 25  | A    |
| 26  | RB    | 27  | C    |
| 26  | RB    | 33  | G    |
| 26  | RB    | 35  | U    |
| 26  | RB    | 40  | U    |
| 26  | RB    | 42  | C    |
| 26  | RB    | 44  | G    |
| 26  | RB    | 45  | A    |
| 26  | RB    | 52  | A    |
| 26  | RB    | 67  | G    |
| 26  | RB    | 73  | A    |
| 26  | RB    | 88  | C    |
| 26  | RB    | 89  | G    |
| 26  | RB    | 108 | C    |
| 26  | RB    | 109 | G    |
| 1   | XA    | 4   | U    |
| 1   | XA    | 5   | U    |
| 1   | XA    | 6   | G    |
| 1   | XA    | 9   | G    |
| 1   | XA    | 22  | G    |
| 1   | XA    | 32  | A    |
| 1   | XA    | 39  | G    |
| 1   | XA    | 47  | C    |
| 1   | XA    | 48  | C    |
| 1   | XA    | 51  | A    |
| 1   | XA    | 54  | C    |
| 1   | XA    | 61  | G    |
| 1   | XA    | 66  | G    |
| 1   | XA    | 72  | C    |
| 1   | XA    | 73  | G    |
| 1   | XA    | 78  | G    |
| 1   | XA    | 96  | U    |
| 1   | XA    | 101 | A    |
| 1   | XA    | 116 | A    |
| 1   | XA    | 120 | A    |
| 1   | XA    | 121 | C    |
| 1   | XA    | 131 | C    |
| 1   | XA    | 163 | C    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | XA           | 169        | C           |
| 1          | XA           | 182        | U           |
| 1          | XA           | 189(C)     | C           |
| 1          | XA           | 189(F)     | U           |
| 1          | XA           | 189(G)     | G           |
| 1          | XA           | 189(H)     | G           |
| 1          | XA           | 189(K)     | U           |
| 1          | XA           | 189(L)     | G           |
| 1          | XA           | 195        | A           |
| 1          | XA           | 197        | A           |
| 1          | XA           | 198        | G           |
| 1          | XA           | 202        | U           |
| 1          | XA           | 203        | U           |
| 1          | XA           | 204        | U           |
| 1          | XA           | 216        | G           |
| 1          | XA           | 244        | U           |
| 1          | XA           | 247        | G           |
| 1          | XA           | 251        | G           |
| 1          | XA           | 266        | G           |
| 1          | XA           | 267        | C           |
| 1          | XA           | 280        | C           |
| 1          | XA           | 281        | G           |
| 1          | XA           | 289        | G           |
| 1          | XA           | 315        | A           |
| 1          | XA           | 316        | G           |
| 1          | XA           | 321        | A           |
| 1          | XA           | 328        | C           |
| 1          | XA           | 329        | A           |
| 1          | XA           | 332        | G           |
| 1          | XA           | 345        | C           |
| 1          | XA           | 347        | G           |
| 1          | XA           | 350        | G           |
| 1          | XA           | 351        | G           |
| 1          | XA           | 352        | C           |
| 1          | XA           | 353        | A           |
| 1          | XA           | 354        | G           |
| 1          | XA           | 356        | A           |
| 1          | XA           | 367        | U           |
| 1          | XA           | 368        | U           |
| 1          | XA           | 372        | C           |
| 1          | XA           | 373        | A           |
| 1          | XA           | 384        | G           |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | XA    | 397 | A    |
| 1   | XA    | 398 | C    |
| 1   | XA    | 406 | G    |
| 1   | XA    | 411 | A    |
| 1   | XA    | 412 | A    |
| 1   | XA    | 413 | G    |
| 1   | XA    | 422 | C    |
| 1   | XA    | 423 | G    |
| 1   | XA    | 424 | G    |
| 1   | XA    | 429 | U    |
| 1   | XA    | 430 | A    |
| 1   | XA    | 439 | A    |
| 1   | XA    | 442 | C    |
| 1   | XA    | 452 | A    |
| 1   | XA    | 453 | A    |
| 1   | XA    | 470 | C    |
| 1   | XA    | 471 | G    |
| 1   | XA    | 477 | A    |
| 1   | XA    | 482 | A    |
| 1   | XA    | 485 | G    |
| 1   | XA    | 486 | U    |
| 1   | XA    | 494 | U    |
| 1   | XA    | 496 | A    |
| 1   | XA    | 498 | U    |
| 1   | XA    | 505 | G    |
| 1   | XA    | 511 | C    |
| 1   | XA    | 518 | C    |
| 1   | XA    | 527 | G    |
| 1   | XA    | 531 | U    |
| 1   | XA    | 532 | A    |
| 1   | XA    | 533 | A    |
| 1   | XA    | 536 | C    |
| 1   | XA    | 545 | C    |
| 1   | XA    | 547 | A    |
| 1   | XA    | 548 | G    |
| 1   | XA    | 559 | A    |
| 1   | XA    | 563 | A    |
| 1   | XA    | 564 | C    |
| 1   | XA    | 572 | A    |
| 1   | XA    | 573 | A    |
| 1   | XA    | 576 | G    |
| 1   | XA    | 577 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | XA    | 579 | G    |
| 1   | XA    | 596 | C    |
| 1   | XA    | 618 | C    |
| 1   | XA    | 630 | G    |
| 1   | XA    | 653 | A    |
| 1   | XA    | 665 | A    |
| 1   | XA    | 687 | A    |
| 1   | XA    | 688 | G    |
| 1   | XA    | 697 | U    |
| 1   | XA    | 702 | A    |
| 1   | XA    | 703 | G    |
| 1   | XA    | 704 | A    |
| 1   | XA    | 724 | G    |
| 1   | XA    | 731 | G    |
| 1   | XA    | 749 | C    |
| 1   | XA    | 755 | G    |
| 1   | XA    | 760 | G    |
| 1   | XA    | 774 | G    |
| 1   | XA    | 777 | A    |
| 1   | XA    | 792 | A    |
| 1   | XA    | 793 | U    |
| 1   | XA    | 794 | A    |
| 1   | XA    | 801 | U    |
| 1   | XA    | 812 | C    |
| 1   | XA    | 813 | U    |
| 1   | XA    | 816 | A    |
| 1   | XA    | 817 | C    |
| 1   | XA    | 818 | G    |
| 1   | XA    | 819 | A    |
| 1   | XA    | 820 | U    |
| 1   | XA    | 821 | G    |
| 1   | XA    | 828 | A    |
| 1   | XA    | 839 | U    |
| 1   | XA    | 840 | C    |
| 1   | XA    | 841 | U    |
| 1   | XA    | 848 | C    |
| 1   | XA    | 855 | G    |
| 1   | XA    | 859 | A    |
| 1   | XA    | 870 | U    |
| 1   | XA    | 874 | G    |
| 1   | XA    | 887 | G    |
| 1   | XA    | 914 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | XA    | 926     | G    |
| 1   | XA    | 927     | G    |
| 1   | XA    | 934     | C    |
| 1   | XA    | 935     | A    |
| 1   | XA    | 960     | U    |
| 1   | XA    | 961     | U    |
| 1   | XA    | 966     | G    |
| 1   | XA    | 968     | A    |
| 1   | XA    | 969     | A    |
| 1   | XA    | 971     | G    |
| 1   | XA    | 972     | C    |
| 1   | XA    | 975     | A    |
| 1   | XA    | 977     | A    |
| 1   | XA    | 980     | C    |
| 1   | XA    | 982     | U    |
| 1   | XA    | 983     | A    |
| 1   | XA    | 991     | U    |
| 1   | XA    | 992     | U    |
| 1   | XA    | 993     | G    |
| 1   | XA    | 1001    | A    |
| 1   | XA    | 1001(A) | G    |
| 1   | XA    | 1005    | A    |
| 1   | XA    | 1006    | C    |
| 1   | XA    | 1007    | C    |
| 1   | XA    | 1008    | C    |
| 1   | XA    | 1009    | G    |
| 1   | XA    | 1020    | U    |
| 1   | XA    | 1024    | G    |
| 1   | XA    | 1025    | U    |
| 1   | XA    | 1026    | G    |
| 1   | XA    | 1029    | C    |
| 1   | XA    | 1030(A) | G    |
| 1   | XA    | 1030(C) | G    |
| 1   | XA    | 1030(D) | A    |
| 1   | XA    | 1031    | G    |
| 1   | XA    | 1033    | G    |
| 1   | XA    | 1034    | G    |
| 1   | XA    | 1036    | G    |
| 1   | XA    | 1038    | C    |
| 1   | XA    | 1039    | C    |
| 1   | XA    | 1042    | G    |
| 1   | XA    | 1053    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | XA    | 1054 | C    |
| 1   | XA    | 1066 | C    |
| 1   | XA    | 1068 | G    |
| 1   | XA    | 1081 | G    |
| 1   | XA    | 1086 | U    |
| 1   | XA    | 1094 | G    |
| 1   | XA    | 1095 | U    |
| 1   | XA    | 1101 | A    |
| 1   | XA    | 1118 | C    |
| 1   | XA    | 1124 | G    |
| 1   | XA    | 1125 | U    |
| 1   | XA    | 1136 | U    |
| 1   | XA    | 1137 | C    |
| 1   | XA    | 1138 | G    |
| 1   | XA    | 1139 | G    |
| 1   | XA    | 1145 | C    |
| 1   | XA    | 1146 | A    |
| 1   | XA    | 1151 | A    |
| 1   | XA    | 1157 | A    |
| 1   | XA    | 1158 | C    |
| 1   | XA    | 1159 | U    |
| 1   | XA    | 1160 | G    |
| 1   | XA    | 1176 | A    |
| 1   | XA    | 1178 | G    |
| 1   | XA    | 1181 | G    |
| 1   | XA    | 1182 | G    |
| 1   | XA    | 1183 | A    |
| 1   | XA    | 1184 | G    |
| 1   | XA    | 1187 | G    |
| 1   | XA    | 1190 | G    |
| 1   | XA    | 1191 | A    |
| 1   | XA    | 1196 | U    |
| 1   | XA    | 1197 | G    |
| 1   | XA    | 1212 | U    |
| 1   | XA    | 1213 | A    |
| 1   | XA    | 1225 | A    |
| 1   | XA    | 1226 | C    |
| 1   | XA    | 1238 | A    |
| 1   | XA    | 1240 | U    |
| 1   | XA    | 1241 | G    |
| 1   | XA    | 1250 | A    |
| 1   | XA    | 1256 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | XA    | 1257    | U    |
| 1   | XA    | 1258    | G    |
| 1   | XA    | 1270    | C    |
| 1   | XA    | 1273    | G    |
| 1   | XA    | 1278    | U    |
| 1   | XA    | 1280    | A    |
| 1   | XA    | 1281    | U    |
| 1   | XA    | 1285    | A    |
| 1   | XA    | 1286    | A    |
| 1   | XA    | 1287    | A    |
| 1   | XA    | 1299    | A    |
| 1   | XA    | 1300    | G    |
| 1   | XA    | 1301    | U    |
| 1   | XA    | 1303    | C    |
| 1   | XA    | 1305    | G    |
| 1   | XA    | 1317    | C    |
| 1   | XA    | 1323    | G    |
| 1   | XA    | 1331    | G    |
| 1   | XA    | 1334    | G    |
| 1   | XA    | 1338    | G    |
| 1   | XA    | 1346    | A    |
| 1   | XA    | 1353    | G    |
| 1   | XA    | 1363    | C    |
| 1   | XA    | 1363(A) | A    |
| 1   | XA    | 1364    | U    |
| 1   | XA    | 1397    | C    |
| 1   | XA    | 1406    | U    |
| 1   | XA    | 1419    | G    |
| 1   | XA    | 1442    | G    |
| 1   | XA    | 1442(B) | A    |
| 1   | XA    | 1443    | G    |
| 1   | XA    | 1446    | U    |
| 1   | XA    | 1447    | A    |
| 1   | XA    | 1452    | C    |
| 1   | XA    | 1456    | G    |
| 1   | XA    | 1457    | G    |
| 1   | XA    | 1493    | A    |
| 1   | XA    | 1494    | G    |
| 1   | XA    | 1497    | G    |
| 1   | XA    | 1499    | A    |
| 1   | XA    | 1502    | A    |
| 1   | XA    | 1503    | A    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | XA    | 1504  | G    |
| 1   | XA    | 1505  | G    |
| 1   | XA    | 1506  | U    |
| 1   | XA    | 1517  | G    |
| 1   | XA    | 1519  | A    |
| 1   | XA    | 1520  | G    |
| 1   | XA    | 1529  | G    |
| 1   | XA    | 1530  | G    |
| 1   | XA    | 1532  | U    |
| 1   | XA    | 1533  | C    |
| 1   | XA    | 1534  | A    |
| 1   | XA    | 1536  | C    |
| 1   | XA    | 1540  | U    |
| 1   | XA    | 1541  | U    |
| 1   | XA    | 1542  | U    |
| 22  | XV    | 13    | C    |
| 22  | XV    | 17(A) | U    |
| 22  | XV    | 18    | G    |
| 22  | XV    | 19    | G    |
| 22  | XV    | 20    | U    |
| 22  | XV    | 21    | A    |
| 22  | XV    | 22    | G    |
| 22  | XV    | 47    | U    |
| 22  | XV    | 48    | C    |
| 22  | XV    | 54    | U    |
| 22  | XV    | 65    | C    |
| 22  | XV    | 76    | A    |
| 22  | XW    | 8     | U    |
| 22  | XW    | 9     | G    |
| 22  | XW    | 10    | G    |
| 22  | XW    | 13    | C    |
| 22  | XW    | 14    | A    |
| 22  | XW    | 15    | G    |
| 22  | XW    | 18    | G    |
| 22  | XW    | 20    | U    |
| 22  | XW    | 21    | A    |
| 22  | XW    | 22    | G    |
| 22  | XW    | 47    | U    |
| 22  | XW    | 48    | C    |
| 22  | XW    | 49    | G    |
| 22  | XW    | 55    | U    |
| 22  | XW    | 57    | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 22         | XW           | 61         | C           |
| 22         | XW           | 66         | C           |
| 22         | XW           | 72         | A           |
| 23         | XX           | 5          | A           |
| 23         | XX           | 11         | U           |
| 23         | XX           | 12         | A           |
| 23         | XX           | 13         | A           |
| 23         | XX           | 14         | A           |
| 23         | XX           | 15         | A           |
| 23         | XX           | 19         | A2M         |
| 23         | XX           | 20         | A2M         |
| 23         | XX           | 21         | A2M         |
| 25         | YA           | 9          | U           |
| 25         | YA           | 15         | G           |
| 25         | YA           | 46         | C           |
| 25         | YA           | 51         | G           |
| 25         | YA           | 55         | G           |
| 25         | YA           | 58         | G           |
| 25         | YA           | 60         | G           |
| 25         | YA           | 69         | C           |
| 25         | YA           | 71         | A           |
| 25         | YA           | 74         | A           |
| 25         | YA           | 75         | G           |
| 25         | YA           | 82         | G           |
| 25         | YA           | 83         | G           |
| 25         | YA           | 95         | G           |
| 25         | YA           | 102        | G           |
| 25         | YA           | 118        | A           |
| 25         | YA           | 119        | A           |
| 25         | YA           | 120        | U           |
| 25         | YA           | 140        | A           |
| 25         | YA           | 154        | G           |
| 25         | YA           | 175        | G           |
| 25         | YA           | 181        | A           |
| 25         | YA           | 182        | A           |
| 25         | YA           | 196        | A           |
| 25         | YA           | 199        | A           |
| 25         | YA           | 215        | G           |
| 25         | YA           | 216        | A           |
| 25         | YA           | 221        | A           |
| 25         | YA           | 222        | A           |
| 25         | YA           | 229        | A           |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | YA    | 233    | A    |
| 25  | YA    | 248    | G    |
| 25  | YA    | 249    | C    |
| 25  | YA    | 252    | G    |
| 25  | YA    | 261    | G    |
| 25  | YA    | 270(B) | A    |
| 25  | YA    | 270(K) | C    |
| 25  | YA    | 270(M) | U    |
| 25  | YA    | 270(O) | U    |
| 25  | YA    | 270(P) | C    |
| 25  | YA    | 270(Z) | U    |
| 25  | YA    | 271(C) | U    |
| 25  | YA    | 271    | G    |
| 25  | YA    | 273(D) | C    |
| 25  | YA    | 274    | G    |
| 25  | YA    | 278    | A    |
| 25  | YA    | 279    | C    |
| 25  | YA    | 283    | A    |
| 25  | YA    | 289    | A    |
| 25  | YA    | 311    | A    |
| 25  | YA    | 324    | A    |
| 25  | YA    | 329    | G    |
| 25  | YA    | 330    | A    |
| 25  | YA    | 332    | A    |
| 25  | YA    | 352    | G    |
| 25  | YA    | 356    | G    |
| 25  | YA    | 361    | G    |
| 25  | YA    | 363    | G    |
| 25  | YA    | 363(A) | A    |
| 25  | YA    | 363(E) | U    |
| 25  | YA    | 363(F) | A    |
| 25  | YA    | 364    | C    |
| 25  | YA    | 372    | G    |
| 25  | YA    | 386    | G    |
| 25  | YA    | 396    | G    |
| 25  | YA    | 407    | G    |
| 25  | YA    | 411    | G    |
| 25  | YA    | 428    | A    |
| 25  | YA    | 444    | C    |
| 25  | YA    | 448    | U    |
| 25  | YA    | 454    | A    |
| 25  | YA    | 456    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | YA    | 470 | A    |
| 25  | YA    | 481 | G    |
| 25  | YA    | 494 | G    |
| 25  | YA    | 504 | U    |
| 25  | YA    | 505 | A    |
| 25  | YA    | 509 | C    |
| 25  | YA    | 512 | G    |
| 25  | YA    | 525 | U    |
| 25  | YA    | 529 | A    |
| 25  | YA    | 530 | G    |
| 25  | YA    | 531 | C    |
| 25  | YA    | 532 | A    |
| 25  | YA    | 533 | G    |
| 25  | YA    | 561 | G    |
| 25  | YA    | 563 | G    |
| 25  | YA    | 571 | A    |
| 25  | YA    | 573 | G    |
| 25  | YA    | 575 | A    |
| 25  | YA    | 586 | A    |
| 25  | YA    | 588 | U    |
| 25  | YA    | 603 | A    |
| 25  | YA    | 607 | U    |
| 25  | YA    | 614 | U    |
| 25  | YA    | 615 | G    |
| 25  | YA    | 617 | G    |
| 25  | YA    | 622 | G    |
| 25  | YA    | 624 | C    |
| 25  | YA    | 625 | G    |
| 25  | YA    | 627 | A    |
| 25  | YA    | 637 | A    |
| 25  | YA    | 645 | C    |
| 25  | YA    | 646 | A    |
| 25  | YA    | 647 | G    |
| 25  | YA    | 670 | A    |
| 25  | YA    | 686 | G    |
| 25  | YA    | 708 | C    |
| 25  | YA    | 722 | A    |
| 25  | YA    | 730 | C    |
| 25  | YA    | 753 | C    |
| 25  | YA    | 764 | A    |
| 25  | YA    | 775 | G    |
| 25  | YA    | 776 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | YA    | 777 | A    |
| 25  | YA    | 782 | A    |
| 25  | YA    | 784 | A    |
| 25  | YA    | 785 | G    |
| 25  | YA    | 789 | A    |
| 25  | YA    | 790 | C    |
| 25  | YA    | 792 | G    |
| 25  | YA    | 805 | G    |
| 25  | YA    | 812 | C    |
| 25  | YA    | 819 | A    |
| 25  | YA    | 827 | U    |
| 25  | YA    | 828 | U    |
| 25  | YA    | 832 | G    |
| 25  | YA    | 848 | G    |
| 25  | YA    | 856 | C    |
| 25  | YA    | 857 | C    |
| 25  | YA    | 859 | G    |
| 25  | YA    | 860 | U    |
| 25  | YA    | 866 | A    |
| 25  | YA    | 878 | A    |
| 25  | YA    | 879 | G    |
| 25  | YA    | 881 | G    |
| 25  | YA    | 882 | G    |
| 25  | YA    | 883 | G    |
| 25  | YA    | 884 | C    |
| 25  | YA    | 886 | C    |
| 25  | YA    | 889 | C    |
| 25  | YA    | 890 | A    |
| 25  | YA    | 893 | C    |
| 25  | YA    | 894 | C    |
| 25  | YA    | 896 | A    |
| 25  | YA    | 897 | C    |
| 25  | YA    | 901 | A    |
| 25  | YA    | 906 | G    |
| 25  | YA    | 907 | U    |
| 25  | YA    | 910 | A    |
| 25  | YA    | 914 | C    |
| 25  | YA    | 917 | A    |
| 25  | YA    | 919 | G    |
| 25  | YA    | 928 | G    |
| 25  | YA    | 932 | G    |
| 25  | YA    | 938 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 941  | A    |
| 25  | YA    | 944  | G    |
| 25  | YA    | 945  | A    |
| 25  | YA    | 946  | G    |
| 25  | YA    | 953  | A    |
| 25  | YA    | 961  | C    |
| 25  | YA    | 973  | A    |
| 25  | YA    | 974  | G    |
| 25  | YA    | 980  | A    |
| 25  | YA    | 983  | A    |
| 25  | YA    | 987  | G    |
| 25  | YA    | 989  | G    |
| 25  | YA    | 990  | A    |
| 25  | YA    | 996  | A    |
| 25  | YA    | 997  | G    |
| 25  | YA    | 998  | C    |
| 25  | YA    | 1000 | A    |
| 25  | YA    | 1010 | A    |
| 25  | YA    | 1011 | G    |
| 25  | YA    | 1012 | U    |
| 25  | YA    | 1013 | C    |
| 25  | YA    | 1022 | G    |
| 25  | YA    | 1023 | U    |
| 25  | YA    | 1025 | G    |
| 25  | YA    | 1026 | U    |
| 25  | YA    | 1033 | U    |
| 25  | YA    | 1044 | G    |
| 25  | YA    | 1045 | A    |
| 25  | YA    | 1046 | A    |
| 25  | YA    | 1047 | G    |
| 25  | YA    | 1049 | C    |
| 25  | YA    | 1051 | G    |
| 25  | YA    | 1060 | U    |
| 25  | YA    | 1061 | U    |
| 25  | YA    | 1070 | A    |
| 25  | YA    | 1086 | A    |
| 25  | YA    | 1087 | G    |
| 25  | YA    | 1088 | A    |
| 25  | YA    | 1089 | G    |
| 25  | YA    | 1095 | A    |
| 25  | YA    | 1096 | A    |
| 25  | YA    | 1122 | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 1128       | A           |
| 25         | YA           | 1130       | U           |
| 25         | YA           | 1135       | C           |
| 25         | YA           | 1136       | G           |
| 25         | YA           | 1139       | G           |
| 25         | YA           | 1142       | U           |
| 25         | YA           | 1143       | A           |
| 25         | YA           | 1155       | A           |
| 25         | YA           | 1173       | G           |
| 25         | YA           | 1174       | A           |
| 25         | YA           | 1175       | U           |
| 25         | YA           | 1176       | G           |
| 25         | YA           | 1177       | A           |
| 25         | YA           | 1178       | C           |
| 25         | YA           | 1180       | C           |
| 25         | YA           | 1195       | G           |
| 25         | YA           | 1218       | C           |
| 25         | YA           | 1220       | A           |
| 25         | YA           | 1236       | G           |
| 25         | YA           | 1247       | A           |
| 25         | YA           | 1248       | G           |
| 25         | YA           | 1250       | G           |
| 25         | YA           | 1253       | A           |
| 25         | YA           | 1255       | U           |
| 25         | YA           | 1256       | G           |
| 25         | YA           | 1262       | A           |
| 25         | YA           | 1265       | A           |
| 25         | YA           | 1271       | G           |
| 25         | YA           | 1272       | A           |
| 25         | YA           | 1276       | A           |
| 25         | YA           | 1281       | G           |
| 25         | YA           | 1289       | C           |
| 25         | YA           | 1300       | U           |
| 25         | YA           | 1301       | A           |
| 25         | YA           | 1303       | G           |
| 25         | YA           | 1314       | C           |
| 25         | YA           | 1319       | G           |
| 25         | YA           | 1329       | U           |
| 25         | YA           | 1352       | U           |
| 25         | YA           | 1359       | A           |
| 25         | YA           | 1360       | A           |
| 25         | YA           | 1365       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 1368       | G           |
| 25         | YA           | 1380       | G           |
| 25         | YA           | 1384       | A           |
| 25         | YA           | 1385       | G           |
| 25         | YA           | 1391       | U           |
| 25         | YA           | 1406       | U           |
| 25         | YA           | 1407       | C           |
| 25         | YA           | 1416       | G           |
| 25         | YA           | 1417       | C           |
| 25         | YA           | 1419       | A           |
| 25         | YA           | 1420       | U           |
| 25         | YA           | 1421       | G           |
| 25         | YA           | 1428       | C           |
| 25         | YA           | 1434       | A           |
| 25         | YA           | 1437       | C           |
| 25         | YA           | 1444(A)    | A           |
| 25         | YA           | 1449       | A           |
| 25         | YA           | 1449(A)    | G           |
| 25         | YA           | 1451       | C           |
| 25         | YA           | 1453       | A           |
| 25         | YA           | 1455       | G           |
| 25         | YA           | 1458       | C           |
| 25         | YA           | 1460       | A           |
| 25         | YA           | 1461       | G           |
| 25         | YA           | 1467       | C           |
| 25         | YA           | 1471       | A           |
| 25         | YA           | 1475       | G           |
| 25         | YA           | 1476       | C           |
| 25         | YA           | 1477       | A           |
| 25         | YA           | 1482       | U           |
| 25         | YA           | 1483       | G           |
| 25         | YA           | 1485       | G           |
| 25         | YA           | 1488       | G           |
| 25         | YA           | 1490       | A           |
| 25         | YA           | 1493       | C           |
| 25         | YA           | 1497       | U           |
| 25         | YA           | 1502       | C           |
| 25         | YA           | 1505       | C           |
| 25         | YA           | 1506       | C           |
| 25         | YA           | 1508       | A           |
| 25         | YA           | 1509       | C           |
| 25         | YA           | 1510       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 1514       | U           |
| 25         | YA           | 1515       | C           |
| 25         | YA           | 1519       | G           |
| 25         | YA           | 1522       | G           |
| 25         | YA           | 1526       | G           |
| 25         | YA           | 1534       | G           |
| 25         | YA           | 1535       | U           |
| 25         | YA           | 1536       | A           |
| 25         | YA           | 1537       | C           |
| 25         | YA           | 1543       | A           |
| 25         | YA           | 1544       | C           |
| 25         | YA           | 1545       | A           |
| 25         | YA           | 1547       | C           |
| 25         | YA           | 1554       | A           |
| 25         | YA           | 1558       | A           |
| 25         | YA           | 1559       | G           |
| 25         | YA           | 1566       | A           |
| 25         | YA           | 1569       | A           |
| 25         | YA           | 1575       | C           |
| 25         | YA           | 1578       | U           |
| 25         | YA           | 1579       | A           |
| 25         | YA           | 1581       | G           |
| 25         | YA           | 1585       | C           |
| 25         | YA           | 1586       | A           |
| 25         | YA           | 1587       | A           |
| 25         | YA           | 1592       | C           |
| 25         | YA           | 1598       | C           |
| 25         | YA           | 1608       | A           |
| 25         | YA           | 1609       | A           |
| 25         | YA           | 1610       | A           |
| 25         | YA           | 1616       | A           |
| 25         | YA           | 1618       | A           |
| 25         | YA           | 1634       | A           |
| 25         | YA           | 1640       | C           |
| 25         | YA           | 1648       | C           |
| 25         | YA           | 1654       | A           |
| 25         | YA           | 1667       | G           |
| 25         | YA           | 1674       | G           |
| 25         | YA           | 1675       | C           |
| 25         | YA           | 1695       | G           |
| 25         | YA           | 1696       | G           |
| 25         | YA           | 1700       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 1701       | A           |
| 25         | YA           | 1703       | G           |
| 25         | YA           | 1725       | G           |
| 25         | YA           | 1729       | A           |
| 25         | YA           | 1733       | G           |
| 25         | YA           | 1735       | C           |
| 25         | YA           | 1742       | C           |
| 25         | YA           | 1750       | G           |
| 25         | YA           | 1754       | C           |
| 25         | YA           | 1756       | G           |
| 25         | YA           | 1763       | G           |
| 25         | YA           | 1764       | G           |
| 25         | YA           | 1773       | A           |
| 25         | YA           | 1780       | A           |
| 25         | YA           | 1791       | A           |
| 25         | YA           | 1800       | C           |
| 25         | YA           | 1801       | G           |
| 25         | YA           | 1816       | G           |
| 25         | YA           | 1820       | U           |
| 25         | YA           | 1829       | A           |
| 25         | YA           | 1835       | G           |
| 25         | YA           | 1838       | C           |
| 25         | YA           | 1839       | G           |
| 25         | YA           | 1847       | A           |
| 25         | YA           | 1848       | A           |
| 25         | YA           | 1858       | G           |
| 25         | YA           | 1869       | G           |
| 25         | YA           | 1870       | C           |
| 25         | YA           | 1872       | A           |
| 25         | YA           | 1878       | G           |
| 25         | YA           | 1881       | C           |
| 25         | YA           | 1882       | C           |
| 25         | YA           | 1888       | G           |
| 25         | YA           | 1889       | A           |
| 25         | YA           | 1896       | G           |
| 25         | YA           | 1900       | A           |
| 25         | YA           | 1903       | G           |
| 25         | YA           | 1905       | C           |
| 25         | YA           | 1906       | G           |
| 25         | YA           | 1912       | A           |
| 25         | YA           | 1913       | A           |
| 25         | YA           | 1914       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 1916       | A           |
| 25         | YA           | 1929       | G           |
| 25         | YA           | 1930       | G           |
| 25         | YA           | 1931       | U           |
| 25         | YA           | 1936       | A           |
| 25         | YA           | 1938       | A           |
| 25         | YA           | 1946       | U           |
| 25         | YA           | 1948       | G           |
| 25         | YA           | 1955       | U           |
| 25         | YA           | 1963       | U           |
| 25         | YA           | 1967       | C           |
| 25         | YA           | 1970       | A           |
| 25         | YA           | 1971       | A           |
| 25         | YA           | 1972       | A           |
| 25         | YA           | 1982       | C           |
| 25         | YA           | 1992       | G           |
| 25         | YA           | 1993       | U           |
| 25         | YA           | 2012       | G           |
| 25         | YA           | 2020       | A           |
| 25         | YA           | 2021       | C           |
| 25         | YA           | 2023       | G           |
| 25         | YA           | 2025       | C           |
| 25         | YA           | 2027       | G           |
| 25         | YA           | 2031       | A           |
| 25         | YA           | 2032       | G           |
| 25         | YA           | 2033       | A           |
| 25         | YA           | 2041       | U           |
| 25         | YA           | 2043       | C           |
| 25         | YA           | 2049       | G           |
| 25         | YA           | 2055       | C           |
| 25         | YA           | 2056       | G           |
| 25         | YA           | 2059       | A           |
| 25         | YA           | 2060       | A           |
| 25         | YA           | 2061       | G           |
| 25         | YA           | 2062       | A           |
| 25         | YA           | 2069       | G           |
| 25         | YA           | 2093       | G           |
| 25         | YA           | 2099       | U           |
| 25         | YA           | 2108       | C           |
| 25         | YA           | 2111       | C           |
| 25         | YA           | 2112       | G           |
| 25         | YA           | 2113       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 2114       | A           |
| 25         | YA           | 2116       | G           |
| 25         | YA           | 2117       | A           |
| 25         | YA           | 2120       | G           |
| 25         | YA           | 2126       | A           |
| 25         | YA           | 2128       | C           |
| 25         | YA           | 2130       | U           |
| 25         | YA           | 2131       | G           |
| 25         | YA           | 2132       | U           |
| 25         | YA           | 2134       | A           |
| 25         | YA           | 2140       | C           |
| 25         | YA           | 2145       | C           |
| 25         | YA           | 2148       | G           |
| 25         | YA           | 2161       | C           |
| 25         | YA           | 2167       | U           |
| 25         | YA           | 2168       | G           |
| 25         | YA           | 2169       | A           |
| 25         | YA           | 2170       | A           |
| 25         | YA           | 2171       | A           |
| 25         | YA           | 2173       | A           |
| 25         | YA           | 2186       | G           |
| 25         | YA           | 2190       | G           |
| 25         | YA           | 2191       | G           |
| 25         | YA           | 2192       | G           |
| 25         | YA           | 2198       | A           |
| 25         | YA           | 2210       | G           |
| 25         | YA           | 2211       | G           |
| 25         | YA           | 2212       | A           |
| 25         | YA           | 2215       | G           |
| 25         | YA           | 2225       | A           |
| 25         | YA           | 2226       | C           |
| 25         | YA           | 2238       | G           |
| 25         | YA           | 2239       | G           |
| 25         | YA           | 2246       | G           |
| 25         | YA           | 2268       | A           |
| 25         | YA           | 2275       | C           |
| 25         | YA           | 2283       | C           |
| 25         | YA           | 2287       | A           |
| 25         | YA           | 2288       | A           |
| 25         | YA           | 2305       | A           |
| 25         | YA           | 2306       | C           |
| 25         | YA           | 2307       | G           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 2308 | G    |
| 25  | YA    | 2309 | A    |
| 25  | YA    | 2312 | U    |
| 25  | YA    | 2319 | G    |
| 25  | YA    | 2320 | A    |
| 25  | YA    | 2325 | G    |
| 25  | YA    | 2327 | A    |
| 25  | YA    | 2336 | A    |
| 25  | YA    | 2343 | C    |
| 25  | YA    | 2344 | U    |
| 25  | YA    | 2345 | G    |
| 25  | YA    | 2347 | C    |
| 25  | YA    | 2350 | C    |
| 25  | YA    | 2354 | G    |
| 25  | YA    | 2383 | G    |
| 25  | YA    | 2385 | C    |
| 25  | YA    | 2394 | C    |
| 25  | YA    | 2402 | C    |
| 25  | YA    | 2406 | U    |
| 25  | YA    | 2423 | U    |
| 25  | YA    | 2425 | A    |
| 25  | YA    | 2428 | G    |
| 25  | YA    | 2429 | G    |
| 25  | YA    | 2430 | A    |
| 25  | YA    | 2434 | A    |
| 25  | YA    | 2435 | A    |
| 25  | YA    | 2439 | A    |
| 25  | YA    | 2440 | C    |
| 25  | YA    | 2441 | C    |
| 25  | YA    | 2448 | A    |
| 25  | YA    | 2450 | A    |
| 25  | YA    | 2465 | C    |
| 25  | YA    | 2468 | G    |
| 25  | YA    | 2469 | A    |
| 25  | YA    | 2472 | G    |
| 25  | YA    | 2475 | C    |
| 25  | YA    | 2476 | A    |
| 25  | YA    | 2478 | A    |
| 25  | YA    | 2484 | G    |
| 25  | YA    | 2490 | G    |
| 25  | YA    | 2494 | G    |
| 25  | YA    | 2502 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | YA    | 2505    | G    |
| 25  | YA    | 2518    | A    |
| 25  | YA    | 2529    | G    |
| 25  | YA    | 2535    | G    |
| 25  | YA    | 2554    | U    |
| 25  | YA    | 2558    | C    |
| 25  | YA    | 2566    | A    |
| 25  | YA    | 2567    | G    |
| 25  | YA    | 2569    | G    |
| 25  | YA    | 2573    | C    |
| 25  | YA    | 2578    | G    |
| 25  | YA    | 2582    | G    |
| 25  | YA    | 2585    | U    |
| 25  | YA    | 2586    | C    |
| 25  | YA    | 2602    | A    |
| 25  | YA    | 2609    | U    |
| 25  | YA    | 2611    | U    |
| 25  | YA    | 2612    | C    |
| 25  | YA    | 2623    | G    |
| 25  | YA    | 2629    | A    |
| 25  | YA    | 2630    | G    |
| 25  | YA    | 2645    | G    |
| 25  | YA    | 2647    | U    |
| 25  | YA    | 2654    | A    |
| 25  | YA    | 2655    | G    |
| 25  | YA    | 2665    | A    |
| 25  | YA    | 2673    | G    |
| 25  | YA    | 2689    | U    |
| 25  | YA    | 2691    | C    |
| 25  | YA    | 2712    | U    |
| 25  | YA    | 2712(A) | A    |
| 25  | YA    | 2713    | A    |
| 25  | YA    | 2724    | C    |
| 25  | YA    | 2726    | U    |
| 25  | YA    | 2732    | G    |
| 25  | YA    | 2733    | A    |
| 25  | YA    | 2734    | A    |
| 25  | YA    | 2748    | A    |
| 25  | YA    | 2750    | A    |
| 25  | YA    | 2751    | G    |
| 25  | YA    | 2752    | C    |
| 25  | YA    | 2754    | U    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | YA           | 2758       | A           |
| 25         | YA           | 2762       | G           |
| 25         | YA           | 2777       | G           |
| 25         | YA           | 2778       | A           |
| 25         | YA           | 2779       | U           |
| 25         | YA           | 2787       | C           |
| 25         | YA           | 2790       | A           |
| 25         | YA           | 2791       | C           |
| 25         | YA           | 2792       | G           |
| 25         | YA           | 2807       | G           |
| 25         | YA           | 2810       | A           |
| 25         | YA           | 2818       | G           |
| 25         | YA           | 2820       | A           |
| 25         | YA           | 2821       | A           |
| 25         | YA           | 2827       | C           |
| 25         | YA           | 2828       | C           |
| 25         | YA           | 2833       | G           |
| 25         | YA           | 2834       | G           |
| 25         | YA           | 2835       | A           |
| 25         | YA           | 2845       | G           |
| 25         | YA           | 2846       | G           |
| 25         | YA           | 2849       | U           |
| 25         | YA           | 2850       | A           |
| 25         | YA           | 2860       | A           |
| 25         | YA           | 2866       | U           |
| 25         | YA           | 2872       | G           |
| 25         | YA           | 2879       | C           |
| 25         | YA           | 2880       | C           |
| 25         | YA           | 2892       | A           |
| 25         | YA           | 2893       | G           |
| 25         | YA           | 2894       | G           |
| 25         | YA           | 2896       | C           |
| 25         | YA           | 2897       | U           |
| 26         | YB           | 7          | G           |
| 26         | YB           | 13         | A           |
| 26         | YB           | 14         | U           |
| 26         | YB           | 15         | A           |
| 26         | YB           | 16         | G           |
| 26         | YB           | 25         | A           |
| 26         | YB           | 32         | C           |
| 26         | YB           | 35         | U           |
| 26         | YB           | 40         | U           |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | YB    | 41  | U    |
| 26  | YB    | 42  | C    |
| 26  | YB    | 44  | G    |
| 26  | YB    | 45  | A    |
| 26  | YB    | 47  | C    |
| 26  | YB    | 56  | G    |
| 26  | YB    | 67  | G    |
| 26  | YB    | 73  | A    |
| 26  | YB    | 81  | G    |
| 26  | YB    | 88  | C    |
| 26  | YB    | 109 | G    |
| 26  | YB    | 119 | A    |

All (175) RNA pucker outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | QA    | 31     | G    |
| 1   | QA    | 60     | A    |
| 1   | QA    | 64     | G    |
| 1   | QA    | 115    | G    |
| 1   | QA    | 181    | G    |
| 1   | QA    | 189(G) | G    |
| 1   | QA    | 197    | A    |
| 1   | QA    | 201    | C    |
| 1   | QA    | 243    | A    |
| 1   | QA    | 250    | A    |
| 1   | QA    | 279    | A    |
| 1   | QA    | 328    | C    |
| 1   | QA    | 329    | A    |
| 1   | QA    | 345    | C    |
| 1   | QA    | 350    | G    |
| 1   | QA    | 353    | A    |
| 1   | QA    | 410    | G    |
| 1   | QA    | 428    | G    |
| 1   | QA    | 429    | U    |
| 1   | QA    | 484    | G    |
| 1   | QA    | 485    | G    |
| 1   | QA    | 496    | A    |
| 1   | QA    | 518    | C    |
| 1   | QA    | 547    | A    |
| 1   | QA    | 560    | U    |
| 1   | QA    | 687    | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | QA    | 748    | C    |
| 1   | QA    | 792    | A    |
| 1   | QA    | 812    | C    |
| 1   | QA    | 839    | U    |
| 1   | QA    | 913    | A    |
| 1   | QA    | 960    | U    |
| 1   | QA    | 992    | U    |
| 1   | QA    | 1004   | A    |
| 1   | QA    | 1033   | G    |
| 1   | QA    | 1038   | C    |
| 1   | QA    | 1065   | U    |
| 1   | QA    | 1067   | A    |
| 1   | QA    | 1137   | C    |
| 1   | QA    | 1182   | G    |
| 1   | QA    | 1297   | C    |
| 1   | QA    | 1300   | G    |
| 1   | QA    | 1346   | A    |
| 1   | QA    | 1347   | G    |
| 1   | QA    | 1498   | U    |
| 1   | QA    | 1532   | U    |
| 22  | QW    | 7      | G    |
| 22  | QW    | 60     | U    |
| 23  | QX    | 9      | G    |
| 23  | QX    | 11     | U    |
| 25  | RA    | 90     | U    |
| 25  | RA    | 119    | A    |
| 25  | RA    | 128    | C    |
| 25  | RA    | 195    | A    |
| 25  | RA    | 227    | A    |
| 25  | RA    | 352    | G    |
| 25  | RA    | 387    | U    |
| 25  | RA    | 404    | C    |
| 25  | RA    | 587    | C    |
| 25  | RA    | 603    | A    |
| 25  | RA    | 614(A) | U    |
| 25  | RA    | 748    | G    |
| 25  | RA    | 752    | A    |
| 25  | RA    | 859    | G    |
| 25  | RA    | 877    | U    |
| 25  | RA    | 883    | G    |
| 25  | RA    | 1022   | G    |
| 25  | RA    | 1085   | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | RA    | 1171 | G    |
| 25  | RA    | 1311 | G    |
| 25  | RA    | 1341 | U    |
| 25  | RA    | 1427 | A    |
| 25  | RA    | 1653 | G    |
| 25  | RA    | 1694 | C    |
| 25  | RA    | 1819 | A    |
| 25  | RA    | 1930 | G    |
| 25  | RA    | 1992 | G    |
| 25  | RA    | 2144 | U    |
| 25  | RA    | 2166 | G    |
| 25  | RA    | 2191 | G    |
| 25  | RA    | 2207 | G    |
| 25  | RA    | 2275 | C    |
| 25  | RA    | 2405 | G    |
| 25  | RA    | 2439 | A    |
| 25  | RA    | 2447 | G    |
| 25  | RA    | 2481 | G    |
| 25  | RA    | 2518 | A    |
| 25  | RA    | 2689 | U    |
| 25  | RA    | 2776 | A    |
| 25  | RA    | 2849 | U    |
| 25  | RA    | 2859 | G    |
| 25  | RA    | 2867 | G    |
| 26  | RB    | 66   | A    |
| 1   | XA    | 5    | U    |
| 1   | XA    | 31   | G    |
| 1   | XA    | 60   | A    |
| 1   | XA    | 93   | G    |
| 1   | XA    | 115  | G    |
| 1   | XA    | 181  | G    |
| 1   | XA    | 197  | A    |
| 1   | XA    | 201  | C    |
| 1   | XA    | 243  | A    |
| 1   | XA    | 250  | A    |
| 1   | XA    | 279  | A    |
| 1   | XA    | 315  | A    |
| 1   | XA    | 328  | C    |
| 1   | XA    | 353  | A    |
| 1   | XA    | 410  | G    |
| 1   | XA    | 428  | G    |
| 1   | XA    | 429  | U    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | XA    | 485   | G    |
| 1   | XA    | 547   | A    |
| 1   | XA    | 687   | A    |
| 1   | XA    | 703   | G    |
| 1   | XA    | 748   | C    |
| 1   | XA    | 792   | A    |
| 1   | XA    | 812   | C    |
| 1   | XA    | 818   | G    |
| 1   | XA    | 913   | A    |
| 1   | XA    | 960   | U    |
| 1   | XA    | 991   | U    |
| 1   | XA    | 992   | U    |
| 1   | XA    | 1004  | A    |
| 1   | XA    | 1033  | G    |
| 1   | XA    | 1038  | C    |
| 1   | XA    | 1065  | U    |
| 1   | XA    | 1067  | A    |
| 1   | XA    | 1137  | C    |
| 1   | XA    | 1300  | G    |
| 1   | XA    | 1498  | U    |
| 1   | XA    | 1532  | U    |
| 22  | XV    | 17(A) | U    |
| 23  | XX    | 20    | A2M  |
| 25  | YA    | 74    | A    |
| 25  | YA    | 101   | G    |
| 25  | YA    | 119   | A    |
| 25  | YA    | 196   | A    |
| 25  | YA    | 528   | A    |
| 25  | YA    | 587   | C    |
| 25  | YA    | 752   | A    |
| 25  | YA    | 856   | C    |
| 25  | YA    | 859   | G    |
| 25  | YA    | 877   | U    |
| 25  | YA    | 883   | G    |
| 25  | YA    | 1022  | G    |
| 25  | YA    | 1085  | A    |
| 25  | YA    | 1171  | G    |
| 25  | YA    | 1275  | A    |
| 25  | YA    | 1300  | U    |
| 25  | YA    | 1379  | A    |
| 25  | YA    | 1427  | A    |
| 25  | YA    | 1558  | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | YA    | 1653 | G    |
| 25  | YA    | 1694 | C    |
| 25  | YA    | 1762 | A    |
| 25  | YA    | 1819 | A    |
| 25  | YA    | 1912 | A    |
| 25  | YA    | 1930 | G    |
| 25  | YA    | 1992 | G    |
| 25  | YA    | 2144 | U    |
| 25  | YA    | 2166 | G    |
| 25  | YA    | 2191 | G    |
| 25  | YA    | 2211 | G    |
| 25  | YA    | 2225 | A    |
| 25  | YA    | 2343 | C    |
| 25  | YA    | 2344 | U    |
| 25  | YA    | 2422 | A    |
| 25  | YA    | 2439 | A    |
| 25  | YA    | 2447 | G    |
| 25  | YA    | 2610 | C    |
| 25  | YA    | 2776 | A    |
| 25  | YA    | 2848 | G    |
| 25  | YA    | 2849 | U    |
| 25  | YA    | 2859 | G    |
| 26  | YB    | 66   | A    |

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |       | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 23  | A2M  | QX    | 19  | 23    | 18,25,26     | 1.01 | 1 (5%)      | 18,36,39    | 2.22 | 3 (16%)     |
| 23  | A2M  | QX    | 20  | 23    | 18,25,26     | 1.13 | 1 (5%)      | 18,36,39    | 1.66 | 1 (5%)      |
| 23  | A2M  | QX    | 21  | 1,23  | 18,25,26     | 1.06 | 1 (5%)      | 18,36,39    | 2.06 | 1 (5%)      |
| 23  | A2M  | XX    | 19  | 56,23 | 18,25,26     | 1.03 | 1 (5%)      | 18,36,39    | 2.32 | 5 (27%)     |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | A2M  | XX    | 20  | 23   | 18,25,26     | 1.10 | 2 (11%)  | 18,36,39    | 2.03 | 2 (11%)  |
| 23  | A2M  | XX    | 21  | 1,23 | 18,25,26     | 1.01 | 1 (5%)   | 18,36,39    | 2.35 | 6 (33%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 23  | A2M  | QX    | 19  | 23    | -       | 0/5/27/28 | 0/3/3/3 |
| 23  | A2M  | QX    | 20  | 23    | -       | 0/5/27/28 | 0/3/3/3 |
| 23  | A2M  | QX    | 21  | 1,23  | -       | 0/5/27/28 | 0/3/3/3 |
| 23  | A2M  | XX    | 19  | 56,23 | -       | 0/5/27/28 | 0/3/3/3 |
| 23  | A2M  | XX    | 20  | 23    | -       | 0/5/27/28 | 0/3/3/3 |
| 23  | A2M  | XX    | 21  | 1,23  | -       | 0/5/27/28 | 0/3/3/3 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 23  | XX    | 20  | A2M  | O4'-C1' | 2.34 | 1.44        | 1.41     |
| 23  | QX    | 19  | A2M  | C5-C4   | 2.87 | 1.47        | 1.40     |
| 23  | XX    | 20  | A2M  | C5-C4   | 2.91 | 1.47        | 1.40     |
| 23  | XX    | 21  | A2M  | C5-C4   | 2.93 | 1.47        | 1.40     |
| 23  | QX    | 21  | A2M  | C5-C4   | 3.00 | 1.47        | 1.40     |
| 23  | XX    | 19  | A2M  | C5-C4   | 3.07 | 1.47        | 1.40     |
| 23  | QX    | 20  | A2M  | C5-C4   | 3.38 | 1.48        | 1.40     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | QX    | 19  | A2M  | N3-C2-N1    | -7.43 | 123.04      | 128.87   |
| 23  | QX    | 21  | A2M  | N3-C2-N1    | -7.00 | 123.37      | 128.87   |
| 23  | XX    | 20  | A2M  | N3-C2-N1    | -6.81 | 123.52      | 128.87   |
| 23  | XX    | 21  | A2M  | N3-C2-N1    | -6.67 | 123.63      | 128.87   |
| 23  | XX    | 19  | A2M  | N3-C2-N1    | -6.53 | 123.74      | 128.87   |
| 23  | QX    | 20  | A2M  | N3-C2-N1    | -5.89 | 124.25      | 128.87   |
| 23  | XX    | 19  | A2M  | C1'-N9-C4   | -4.97 | 121.26      | 126.81   |
| 23  | QX    | 19  | A2M  | C1'-N9-C4   | -3.95 | 122.39      | 126.81   |
| 23  | XX    | 21  | A2M  | C4'-O4'-C1' | -3.81 | 105.60      | 109.64   |
| 23  | XX    | 21  | A2M  | C1'-N9-C4   | -3.16 | 123.28      | 126.81   |
| 23  | XX    | 19  | A2M  | C2'-C1'-N9  | -2.23 | 107.12      | 113.48   |
| 23  | XX    | 19  | A2M  | O2'-C2'-C3' | 2.02  | 116.43      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 23  | XX    | 21  | A2M  | C2-N1-C6    | 2.13 | 122.57      | 118.77   |
| 23  | QX    | 19  | A2M  | C2-N1-C6    | 2.13 | 122.58      | 118.77   |
| 23  | XX    | 21  | A2M  | O4'-C1'-N9  | 2.33 | 112.51      | 108.11   |
| 23  | XX    | 21  | A2M  | O2'-C2'-C3' | 2.77 | 118.36      | 111.23   |
| 23  | XX    | 19  | A2M  | O4'-C1'-N9  | 3.20 | 114.14      | 108.11   |
| 23  | XX    | 20  | A2M  | O4'-C1'-N9  | 3.43 | 114.59      | 108.11   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | QX    | 19  | A2M  | 1       | 0            |
| 23  | QX    | 21  | A2M  | 2       | 0            |
| 23  | XX    | 20  | A2M  | 2       | 0            |
| 23  | XX    | 21  | A2M  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1312 ligands modelled in this entry, 1312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | QA    | 1511/1522 (99%) | -0.00  | 42 (2%) 56 52 | 39, 80, 190, 435      | 0     |
| 1   | XA    | 1508/1522 (99%) | -0.02  | 40 (2%) 58 53 | 27, 78, 175, 487      | 0     |
| 2   | QB    | 236/256 (92%)   | 0.55   | 27 (11%) 7 7  | 58, 138, 241, 336     | 0     |
| 2   | XB    | 236/256 (92%)   | 0.31   | 20 (8%) 13 13 | 52, 119, 215, 332     | 0     |
| 3   | QC    | 206/239 (86%)   | 0.41   | 15 (7%) 18 17 | 61, 111, 200, 469     | 0     |
| 3   | XC    | 206/239 (86%)   | 0.25   | 13 (6%) 23 22 | 44, 103, 197, 564     | 0     |
| 4   | QD    | 208/209 (99%)   | -0.18  | 3 (1%) 78 73  | 35, 66, 119, 173      | 0     |
| 4   | XD    | 208/209 (99%)   | 0.04   | 6 (2%) 55 50  | 41, 82, 132, 198      | 0     |
| 5   | QE    | 154/162 (95%)   | -0.08  | 2 (1%) 79 74  | 34, 74, 138, 244      | 0     |
| 5   | XE    | 154/162 (95%)   | -0.02  | 5 (3%) 51 47  | 31, 68, 144, 340      | 0     |
| 6   | QF    | 101/101 (100%)  | 0.35   | 4 (3%) 42 37  | 58, 117, 161, 183     | 0     |
| 6   | XF    | 101/101 (100%)  | -0.15  | 0 100 100     | 29, 68, 110, 175      | 0     |
| 7   | QG    | 155/156 (99%)   | 0.31   | 13 (8%) 14 13 | 80, 130, 214, 347     | 0     |
| 7   | XG    | 155/156 (99%)   | 0.16   | 9 (5%) 26 24  | 54, 101, 179, 252     | 0     |
| 8   | QH    | 138/138 (100%)  | -0.20  | 1 (0%) 89 85  | 41, 81, 119, 179      | 0     |
| 8   | XH    | 138/138 (100%)  | -0.08  | 0 100 100     | 48, 79, 128, 182      | 0     |
| 9   | QI    | 128/128 (100%)  | 0.89   | 21 (16%) 2 2  | 78, 156, 267, 359     | 0     |
| 9   | XI    | 128/128 (100%)  | 0.54   | 12 (9%) 11 11 | 61, 115, 202, 350     | 0     |
| 10  | QJ    | 99/105 (94%)    | 1.01   | 18 (18%) 2 2  | 74, 149, 278, 339     | 0     |
| 10  | XJ    | 99/105 (94%)    | 0.64   | 7 (7%) 19 18  | 63, 133, 253, 371     | 0     |
| 11  | QK    | 121/129 (93%)   | 0.53   | 10 (8%) 14 13 | 43, 102, 182, 301     | 0     |
| 11  | XK    | 121/129 (93%)   | 0.05   | 3 (2%) 61 55  | 32, 71, 159, 258      | 0     |
| 12  | QL    | 125/132 (94%)   | -0.06  | 1 (0%) 87 83  | 27, 62, 103, 271      | 0     |
| 12  | XL    | 125/132 (94%)   | -0.04  | 3 (2%) 62 57  | 30, 64, 103, 263      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13  | QM    | 118/126 (93%)   | 0.56   | 6 (5%) 32 28   | 75, 133, 248, 348     | 0     |
| 13  | XM    | 118/126 (93%)   | 0.36   | 7 (5%) 26 23   | 64, 114, 183, 467     | 0     |
| 14  | QN    | 60/61 (98%)     | 0.80   | 7 (11%) 6 6    | 79, 110, 169, 205     | 0     |
| 14  | XN    | 60/61 (98%)     | 0.55   | 4 (6%) 21 20   | 60, 93, 133, 240      | 0     |
| 15  | QO    | 88/89 (98%)     | 0.05   | 0 100 100      | 37, 86, 136, 170      | 0     |
| 15  | XO    | 88/89 (98%)     | -0.11  | 0 100 100      | 34, 74, 110, 161      | 0     |
| 16  | QP    | 84/88 (95%)     | -0.22  | 1 (1%) 81 75   | 38, 68, 111, 260      | 0     |
| 16  | XP    | 84/88 (95%)     | 0.26   | 1 (1%) 81 75   | 63, 90, 138, 347      | 0     |
| 17  | QQ    | 100/105 (95%)   | 0.01   | 2 (2%) 68 62   | 33, 79, 110, 133      | 0     |
| 17  | XQ    | 100/105 (95%)   | 0.12   | 1 (1%) 84 79   | 35, 82, 118, 188      | 0     |
| 18  | QR    | 71/88 (80%)     | 0.33   | 4 (5%) 28 25   | 64, 114, 191, 248     | 0     |
| 18  | XR    | 71/88 (80%)     | 0.13   | 3 (4%) 40 35   | 33, 66, 181, 270      | 0     |
| 19  | QS    | 82/93 (88%)     | 0.73   | 10 (12%) 5 5   | 78, 148, 306, 418     | 0     |
| 19  | XS    | 82/93 (88%)     | 0.63   | 4 (4%) 33 29   | 57, 126, 215, 401     | 0     |
| 20  | QT    | 99/106 (93%)    | 0.15   | 3 (3%) 54 49   | 54, 85, 160, 222      | 0     |
| 20  | XT    | 99/106 (93%)    | 0.29   | 4 (4%) 42 37   | 61, 107, 176, 212     | 0     |
| 21  | QU    | 25/27 (92%)     | 1.99   | 12 (48%) 0 0   | 94, 130, 197, 278     | 0     |
| 21  | XU    | 25/27 (92%)     | 1.38   | 7 (28%) 1 1    | 74, 113, 170, 194     | 0     |
| 22  | QV    | 77/77 (100%)    | 0.28   | 1 (1%) 79 74   | 46, 83, 132, 187      | 0     |
| 22  | QW    | 77/77 (100%)    | 3.43   | 63 (81%) 0 0   | 86, 279, 383, 409     | 0     |
| 22  | XV    | 77/77 (100%)    | -0.13  | 1 (1%) 79 74   | 42, 79, 123, 172      | 0     |
| 22  | XW    | 77/77 (100%)    | 3.19   | 54 (70%) 0 0   | 115, 271, 335, 411    | 0     |
| 23  | QX    | 17/25 (68%)     | 2.50   | 13 (76%) 0 0   | 53, 218, 306, 334     | 0     |
| 23  | XX    | 17/25 (68%)     | 2.30   | 9 (52%) 0 0    | 45, 237, 354, 390     | 0     |
| 24  | QY    | 91/117 (77%)    | 1.08   | 14 (15%) 3 3   | 83, 126, 163, 188     | 0     |
| 24  | XY    | 91/117 (77%)    | 1.25   | 17 (18%) 2 2   | 82, 127, 165, 185     | 0     |
| 25  | RA    | 2891/2916 (99%) | 0.11   | 159 (5%) 29 26 | 20, 56, 239, 588      | 0     |
| 25  | YA    | 2875/2916 (98%) | 0.05   | 150 (5%) 31 28 | 20, 54, 248, 583      | 0     |
| 26  | RB    | 122/124 (98%)   | 0.05   | 1 (0%) 87 83   | 46, 96, 148, 214      | 0     |
| 26  | YB    | 122/124 (98%)   | -0.01  | 1 (0%) 87 83   | 55, 86, 136, 215      | 0     |
| 27  | RD    | 272/276 (98%)   | -0.11  | 4 (1%) 76 71   | 17, 54, 102, 322      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 27  | YD    | 272/276 (98%)  | -0.27  | 1 (0%) 93 91  | 12, 35, 83, 212       | 0     |
| 28  | RE    | 205/206 (99%)  | 0.12   | 6 (2%) 55 50  | 25, 73, 159, 362      | 0     |
| 28  | YE    | 205/206 (99%)  | 0.11   | 6 (2%) 55 50  | 26, 73, 168, 563      | 0     |
| 29  | RF    | 208/210 (99%)  | -0.12  | 8 (3%) 44 39  | 13, 44, 168, 316      | 0     |
| 29  | YF    | 208/210 (99%)  | 0.03   | 10 (4%) 34 31 | 22, 67, 240, 535      | 0     |
| 30  | RG    | 181/182 (99%)  | 0.26   | 5 (2%) 56 52  | 62, 110, 161, 194     | 0     |
| 30  | YG    | 181/182 (99%)  | 0.13   | 3 (1%) 73 67  | 42, 97, 165, 199      | 0     |
| 31  | RH    | 170/180 (94%)  | 1.34   | 38 (22%) 1 1  | 59, 182, 468, 582     | 0     |
| 31  | YH    | 170/180 (94%)  | 0.95   | 36 (21%) 1 1  | 58, 146, 370, 574     | 0     |
| 32  | RI    | 146/148 (98%)  | 0.47   | 7 (4%) 34 31  | 51, 113, 183, 290     | 0     |
| 32  | YI    | 146/148 (98%)  | 0.35   | 6 (4%) 41 36  | 36, 92, 188, 341      | 0     |
| 33  | RN    | 138/140 (98%)  | -0.15  | 0 100 100     | 25, 75, 121, 188      | 0     |
| 33  | YN    | 138/140 (98%)  | -0.05  | 1 (0%) 89 85  | 26, 81, 141, 196      | 0     |
| 34  | RO    | 122/122 (100%) | -0.38  | 0 100 100     | 26, 58, 90, 120       | 0     |
| 34  | YO    | 122/122 (100%) | -0.37  | 0 100 100     | 27, 58, 91, 116       | 0     |
| 35  | RP    | 150/150 (100%) | 0.02   | 3 (2%) 68 62  | 19, 68, 152, 324      | 0     |
| 35  | YP    | 150/150 (100%) | 0.14   | 6 (4%) 42 37  | 27, 66, 149, 278      | 0     |
| 36  | RQ    | 140/141 (99%)  | 0.02   | 4 (2%) 55 50  | 30, 70, 115, 294      | 0     |
| 36  | YQ    | 139/141 (98%)  | 0.04   | 2 (1%) 78 73  | 35, 70, 127, 273      | 0     |
| 37  | RR    | 117/118 (99%)  | -0.20  | 0 100 100     | 26, 65, 100, 156      | 0     |
| 37  | YR    | 117/118 (99%)  | -0.12  | 0 100 100     | 33, 65, 115, 161      | 0     |
| 38  | RS    | 111/112 (99%)  | 0.29   | 6 (5%) 29 27  | 59, 112, 201, 486     | 0     |
| 38  | YS    | 111/112 (99%)  | 0.28   | 3 (2%) 58 53  | 54, 93, 171, 315      | 0     |
| 39  | RT    | 137/146 (93%)  | -0.10  | 6 (4%) 38 34  | 36, 78, 172, 561      | 0     |
| 39  | YT    | 137/146 (93%)  | 0.28   | 11 (8%) 15 14 | 29, 80, 263, 460      | 0     |
| 40  | RU    | 117/118 (99%)  | -0.18  | 3 (2%) 59 54  | 20, 56, 126, 223      | 0     |
| 40  | YU    | 117/118 (99%)  | 0.06   | 2 (1%) 73 67  | 32, 74, 147, 342      | 0     |
| 41  | RV    | 101/101 (100%) | -0.08  | 3 (2%) 54 49  | 23, 79, 142, 406      | 0     |
| 41  | YV    | 101/101 (100%) | 0.34   | 3 (2%) 54 49  | 27, 102, 149, 576     | 0     |
| 42  | RW    | 113/113 (100%) | -0.15  | 0 100 100     | 23, 53, 113, 248      | 0     |
| 42  | YW    | 113/113 (100%) | -0.00  | 4 (3%) 48 42  | 26, 61, 118, 368      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 43  | RX    | 92/96 (95%)       | -0.04  | 1 (1%) 82 77    | 37, 69, 114, 140      | 0     |
| 43  | YX    | 92/96 (95%)       | -0.18  | 1 (1%) 82 77    | 26, 55, 107, 126      | 0     |
| 44  | RY    | 102/110 (92%)     | 0.77   | 13 (12%) 5 5    | 33, 78, 230, 539      | 0     |
| 44  | YY    | 102/110 (92%)     | 0.77   | 16 (15%) 3 3    | 40, 95, 248, 579      | 0     |
| 45  | RZ    | 176/206 (85%)     | 0.45   | 13 (7%) 17 17   | 54, 109, 230, 333     | 0     |
| 45  | YZ    | 183/206 (88%)     | 0.37   | 14 (7%) 16 16   | 55, 111, 190, 333     | 0     |
| 46  | R0    | 83/85 (97%)       | 0.26   | 6 (7%) 18 17    | 30, 69, 179, 363      | 0     |
| 46  | Y0    | 83/85 (97%)       | 0.28   | 4 (4%) 34 31    | 29, 70, 166, 209      | 0     |
| 47  | R1    | 97/98 (98%)       | 0.39   | 5 (5%) 31 28    | 27, 64, 206, 399      | 0     |
| 47  | Y1    | 97/98 (98%)       | 0.20   | 8 (8%) 14 13    | 17, 46, 207, 422      | 0     |
| 48  | R2    | 69/72 (95%)       | 0.11   | 2 (2%) 55 50    | 35, 87, 189, 288      | 0     |
| 48  | Y2    | 69/72 (95%)       | -0.20  | 1 (1%) 78 73    | 28, 69, 119, 233      | 0     |
| 49  | R3    | 59/60 (98%)       | 0.15   | 2 (3%) 49 44    | 36, 63, 116, 167      | 0     |
| 49  | Y3    | 59/60 (98%)       | 0.05   | 1 (1%) 73 67    | 39, 80, 135, 184      | 0     |
| 50  | R4    | 70/71 (98%)       | 1.29   | 19 (27%) 1 1    | 105, 280, 598, 608    | 0     |
| 50  | Y4    | 70/71 (98%)       | 1.53   | 21 (30%) 1 1    | 92, 189, 571, 588     | 0     |
| 51  | R5    | 59/60 (98%)       | 0.36   | 6 (10%) 9 9     | 21, 60, 201, 299      | 0     |
| 51  | Y5    | 57/60 (95%)       | 0.37   | 5 (8%) 12 12    | 15, 71, 193, 303      | 0     |
| 52  | R6    | 48/54 (88%)       | 1.83   | 19 (39%) 0 0    | 71, 128, 199, 285     | 0     |
| 52  | Y6    | 48/54 (88%)       | 1.66   | 18 (37%) 0 1    | 60, 111, 181, 219     | 0     |
| 53  | R7    | 49/49 (100%)      | -0.19  | 0 100 100       | 15, 36, 127, 208      | 0     |
| 53  | Y7    | 49/49 (100%)      | -0.14  | 2 (4%) 41 36    | 10, 29, 97, 215       | 0     |
| 54  | R8    | 64/65 (98%)       | 0.10   | 2 (3%) 52 48    | 22, 50, 116, 225      | 0     |
| 54  | Y8    | 64/65 (98%)       | 0.30   | 3 (4%) 35 32    | 22, 52, 96, 236       | 0     |
| 55  | R9    | 37/37 (100%)      | 3.11   | 26 (70%) 0 0    | 99, 140, 190, 246     | 0     |
| 55  | Y9    | 36/37 (97%)       | 4.31   | 33 (91%) 0 0    | 88, 155, 219, 248     | 0     |
| All | All   | 21218/21844 (97%) | 0.19   | 1262 (5%) 26 23 | 10, 78, 219, 608      | 0     |

All (1262) RSRZ outliers are listed below:

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 25  | RA    | 2801(A) | A    | 18.9 |
| 25  | RA    | 1075    | C    | 13.8 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | RA    | 2801 | A    | 13.7 |
| 25  | RA    | 2169 | A    | 13.4 |
| 25  | YA    | 2798 | C    | 13.3 |
| 25  | RA    | 1076 | C    | 13.2 |
| 25  | YA    | 2799 | A    | 13.1 |
| 25  | YA    | 2114 | A    | 12.6 |
| 25  | RA    | 1077 | A    | 12.5 |
| 25  | YA    | 1065 | U    | 11.8 |
| 25  | RA    | 1089 | G    | 11.7 |
| 25  | RA    | 2139 | C    | 11.6 |
| 25  | RA    | 1057 | A    | 11.3 |
| 9   | QI    | 1    | MET  | 11.1 |
| 44  | RY    | 49   | VAL  | 11.1 |
| 25  | RA    | 2167 | U    | 11.0 |
| 25  | RA    | 2796 | U    | 10.7 |
| 25  | YA    | 2127 | G    | 10.7 |
| 25  | RA    | 1066 | U    | 10.4 |
| 44  | RY    | 48   | ALA  | 10.4 |
| 25  | YA    | 2115 | G    | 10.3 |
| 22  | QW    | 59   | A    | 10.3 |
| 1   | XA    | 1026 | G    | 10.0 |
| 55  | R9    | 1    | MET  | 9.8  |
| 45  | RZ    | 153  | SER  | 9.8  |
| 28  | RE    | 68   | ALA  | 9.7  |
| 55  | Y9    | 34   | GLN  | 9.7  |
| 55  | Y9    | 32   | HIS  | 9.6  |
| 28  | YE    | 204  | ALA  | 9.6  |
| 25  | YA    | 2801 | A    | 9.5  |
| 47  | Y1    | 95   | LEU  | 9.3  |
| 25  | RA    | 1078 | U    | 9.2  |
| 11  | QK    | 9    | LYS  | 8.8  |
| 29  | YF    | 1    | MET  | 8.8  |
| 25  | RA    | 2116 | G    | 8.7  |
| 1   | QA    | 1542 | U    | 8.7  |
| 55  | Y9    | 29   | ASN  | 8.7  |
| 47  | R1    | 95   | LEU  | 8.6  |
| 25  | RA    | 1099 | G    | 8.4  |
| 22  | XW    | 6    | G    | 8.4  |
| 44  | RY    | 50   | ARG  | 8.4  |
| 3   | XC    | 80   | GLY  | 8.3  |
| 22  | XW    | 5    | G    | 8.3  |
| 25  | YA    | 1068 | G    | 8.3  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 50  | Y4    | 66      | SER  | 8.2  |
| 25  | RA    | 1096    | A    | 8.2  |
| 28  | RE    | 204     | ALA  | 8.2  |
| 25  | YA    | 1536    | A    | 8.2  |
| 25  | RA    | 2160    | G    | 8.2  |
| 25  | RA    | 2802    | G    | 8.2  |
| 25  | YA    | 2176    | A    | 8.2  |
| 22  | XW    | 20      | U    | 8.1  |
| 31  | RH    | 2       | SER  | 8.1  |
| 22  | XW    | 7       | G    | 8.0  |
| 25  | RA    | 2795    | G    | 8.0  |
| 22  | QW    | 16      | C    | 8.0  |
| 31  | RH    | 33      | LEU  | 8.0  |
| 50  | Y4    | 47      | GLN  | 8.0  |
| 25  | YA    | 1074    | G    | 7.9  |
| 25  | YA    | 2172    | U    | 7.9  |
| 25  | YA    | 1093    | G    | 7.7  |
| 28  | YE    | 205     | ALA  | 7.7  |
| 25  | YA    | 2131    | G    | 7.7  |
| 29  | RF    | 208     | GLY  | 7.7  |
| 22  | QW    | 47      | U    | 7.7  |
| 25  | YA    | 1537    | C    | 7.7  |
| 25  | RA    | 1083    | U    | 7.6  |
| 25  | RA    | 2125    | G    | 7.6  |
| 1   | XA    | 1030(C) | G    | 7.6  |
| 44  | YY    | 54      | LYS  | 7.5  |
| 55  | R9    | 34      | GLN  | 7.4  |
| 31  | RH    | 25      | LYS  | 7.4  |
| 25  | YA    | 1073    | A    | 7.4  |
| 25  | YA    | 1099    | G    | 7.4  |
| 22  | XW    | 36      | U    | 7.4  |
| 25  | YA    | 1078    | U    | 7.3  |
| 25  | RA    | 1081    | U    | 7.3  |
| 31  | RH    | 43      | VAL  | 7.3  |
| 1   | XA    | 1025    | U    | 7.3  |
| 22  | XW    | 34      | C    | 7.3  |
| 25  | YA    | 2173    | A    | 7.2  |
| 55  | Y9    | 9       | ARG  | 7.2  |
| 31  | RH    | 32      | GLU  | 7.1  |
| 22  | QW    | 19      | G    | 7.1  |
| 25  | RA    | 1074    | G    | 7.1  |
| 31  | YH    | 2       | SER  | 7.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | YA    | 1066 | U    | 7.1  |
| 25  | YA    | 2169 | A    | 7.1  |
| 22  | XW    | 16   | C    | 7.1  |
| 31  | YH    | 81   | GLU  | 7.1  |
| 25  | YA    | 1060 | U    | 7.0  |
| 3   | QC    | 78   | GLY  | 7.0  |
| 25  | RA    | 2165 | G    | 7.0  |
| 25  | YA    | 2117 | A    | 7.0  |
| 25  | RA    | 2799 | C    | 7.0  |
| 1   | XA    | 1031 | G    | 7.0  |
| 1   | XA    | 1182 | G    | 6.9  |
| 3   | QC    | 79   | ARG  | 6.9  |
| 5   | XE    | 2    | PRO  | 6.9  |
| 20  | QT    | 106  | ALA  | 6.9  |
| 11  | QK    | 128  | ALA  | 6.9  |
| 1   | XA    | 3    | G    | 6.8  |
| 23  | QX    | 3    | C    | 6.8  |
| 2   | QB    | 37   | ASN  | 6.8  |
| 25  | RA    | 1065 | U    | 6.7  |
| 21  | QU    | 18   | TYR  | 6.7  |
| 16  | XP    | 84   | ALA  | 6.7  |
| 25  | YA    | 1075 | C    | 6.7  |
| 25  | RA    | 1068 | G    | 6.7  |
| 25  | RA    | 2135 | A    | 6.6  |
| 55  | Y9    | 10   | ILE  | 6.6  |
| 25  | RA    | 1536 | A    | 6.6  |
| 22  | QW    | 17   | C    | 6.6  |
| 47  | R1    | 94   | LEU  | 6.5  |
| 29  | YF    | 11   | VAL  | 6.5  |
| 25  | RA    | 2157 | G    | 6.5  |
| 29  | RF    | 11   | VAL  | 6.5  |
| 48  | R2    | 43   | GLN  | 6.5  |
| 25  | RA    | 2173 | A    | 6.4  |
| 22  | QW    | 48   | C    | 6.4  |
| 44  | YY    | 48   | ALA  | 6.4  |
| 25  | RA    | 2138 | C    | 6.4  |
| 22  | XW    | 62   | C    | 6.4  |
| 25  | YA    | 1070 | A    | 6.3  |
| 44  | YY    | 49   | VAL  | 6.3  |
| 25  | YA    | 2123 | G    | 6.3  |
| 22  | QW    | 6    | G    | 6.3  |
| 25  | YA    | 2108 | C    | 6.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | YA    | 2151 | G    | 6.2  |
| 1   | QA    | 89   | C    | 6.2  |
| 25  | YA    | 2119 | A    | 6.2  |
| 22  | XW    | 13   | C    | 6.2  |
| 3   | XC    | 79   | ARG  | 6.1  |
| 39  | YT    | 137  | LYS  | 6.1  |
| 25  | YA    | 2141 | G    | 6.1  |
| 11  | XK    | 128  | ALA  | 6.1  |
| 55  | Y9    | 14   | CYS  | 6.1  |
| 25  | YA    | 2797 | U    | 6.1  |
| 2   | QB    | 6    | THR  | 6.1  |
| 25  | RA    | 2168 | G    | 6.0  |
| 25  | YA    | 2116 | G    | 6.0  |
| 22  | QW    | 58   | A    | 6.0  |
| 39  | YT    | 2    | ASN  | 6.0  |
| 22  | XW    | 35   | A    | 5.9  |
| 12  | QL    | 129  | ALA  | 5.9  |
| 9   | XI    | 1    | MET  | 5.9  |
| 29  | YF    | 12   | LEU  | 5.9  |
| 25  | RA    | 2803 | C    | 5.9  |
| 25  | RA    | 2895 | U    | 5.8  |
| 11  | QK    | 129  | SER  | 5.8  |
| 22  | QW    | 34   | C    | 5.8  |
| 25  | YA    | 1080 | C    | 5.8  |
| 39  | YT    | 133  | GLU  | 5.8  |
| 22  | XW    | 61   | C    | 5.8  |
| 25  | RA    | 2126 | A    | 5.8  |
| 25  | RA    | 1093 | G    | 5.8  |
| 35  | RP    | 150  | ALA  | 5.8  |
| 22  | XW    | 58   | A    | 5.8  |
| 18  | XR    | 88   | LYS  | 5.8  |
| 50  | R4    | 71   | ARG  | 5.8  |
| 25  | YA    | 2795 | G    | 5.7  |
| 22  | QW    | 33   | U    | 5.7  |
| 25  | YA    | 2138 | C    | 5.7  |
| 55  | Y9    | 36   | GLN  | 5.7  |
| 25  | YA    | 1061 | U    | 5.7  |
| 50  | Y4    | 12   | ALA  | 5.7  |
| 22  | XW    | 18   | G    | 5.7  |
| 25  | YA    | 1535 | U    | 5.7  |
| 25  | YA    | 2163 | C    | 5.6  |
| 47  | R1    | 98   | LEU  | 5.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 44  | RY    | 47   | LYS  | 5.6  |
| 22  | XW    | 47   | U    | 5.6  |
| 25  | RA    | 1067 | A    | 5.6  |
| 28  | RE    | 205  | ALA  | 5.6  |
| 31  | RH    | 34   | GLU  | 5.6  |
| 25  | YA    | 2110 | G    | 5.6  |
| 31  | RH    | 31   | GLY  | 5.6  |
| 39  | YT    | 129  | ARG  | 5.5  |
| 25  | YA    | 1095 | A    | 5.5  |
| 25  | RA    | 2119 | A    | 5.5  |
| 51  | Y5    | 54   | GLY  | 5.5  |
| 1   | XA    | 1030 | C    | 5.5  |
| 25  | YA    | 1094 | U    | 5.5  |
| 22  | XW    | 73   | A    | 5.4  |
| 25  | RA    | 2127 | G    | 5.4  |
| 46  | Y0    | 6    | GLY  | 5.4  |
| 25  | RA    | 2804 | C    | 5.4  |
| 25  | YA    | 1087 | G    | 5.4  |
| 25  | RA    | 1082 | U    | 5.4  |
| 25  | RA    | 2156 | G    | 5.4  |
| 12  | XL    | 129  | ALA  | 5.4  |
| 44  | YY    | 58   | GLY  | 5.4  |
| 55  | Y9    | 25   | VAL  | 5.4  |
| 55  | Y9    | 11   | CYS  | 5.4  |
| 18  | XR    | 19   | LYS  | 5.4  |
| 23  | XX    | 4    | A    | 5.3  |
| 25  | YA    | 1057 | A    | 5.3  |
| 54  | Y8    | 65   | GLU  | 5.3  |
| 10  | QJ    | 33   | GLN  | 5.3  |
| 25  | RA    | 1064 | C    | 5.3  |
| 50  | Y4    | 65   | ASP  | 5.3  |
| 25  | YA    | 2892 | A    | 5.3  |
| 7   | QG    | 82   | GLY  | 5.3  |
| 50  | Y4    | 39   | CYS  | 5.3  |
| 25  | YA    | 2803 | C    | 5.3  |
| 2   | QB    | 16   | HIS  | 5.3  |
| 22  | QW    | 7    | G    | 5.2  |
| 52  | R6    | 19   | ARG  | 5.2  |
| 46  | Y0    | 3    | HIS  | 5.2  |
| 25  | RA    | 2794 | C    | 5.2  |
| 45  | YZ    | 159  | PRO  | 5.2  |
| 55  | Y9    | 28   | GLU  | 5.2  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 7   | QG    | 3       | ARG  | 5.2  |
| 31  | RH    | 99      | VAL  | 5.2  |
| 22  | QW    | 62      | C    | 5.2  |
| 1   | QA    | 1446    | U    | 5.2  |
| 25  | YA    | 2160    | G    | 5.2  |
| 25  | YA    | 2132    | U    | 5.2  |
| 25  | YA    | 1079    | C    | 5.1  |
| 1   | QA    | 1030    | C    | 5.1  |
| 2   | QB    | 123     | ALA  | 5.1  |
| 11  | QK    | 12      | ARG  | 5.1  |
| 50  | Y4    | 71      | ARG  | 5.1  |
| 38  | YS    | 111     | GLU  | 5.1  |
| 29  | RF    | 12      | LEU  | 5.0  |
| 55  | R9    | 36      | GLN  | 5.0  |
| 22  | QW    | 35      | A    | 5.0  |
| 47  | Y1    | 96      | LYS  | 5.0  |
| 25  | YA    | 1064    | C    | 5.0  |
| 5   | XE    | 154     | GLY  | 5.0  |
| 55  | Y9    | 15      | LYS  | 5.0  |
| 25  | YA    | 2113    | U    | 5.0  |
| 25  | RA    | 1072    | C    | 5.0  |
| 25  | RA    | 2153    | G    | 5.0  |
| 25  | YA    | 1059    | G    | 5.0  |
| 32  | YI    | 143     | SER  | 5.0  |
| 25  | YA    | 2159    | G    | 4.9  |
| 25  | RA    | 2629    | A    | 4.9  |
| 46  | R0    | 85      | ALA  | 4.9  |
| 31  | RH    | 103     | LEU  | 4.9  |
| 13  | QM    | 119     | GLY  | 4.9  |
| 22  | QW    | 60      | U    | 4.9  |
| 31  | RH    | 28      | GLY  | 4.9  |
| 46  | R0    | 8       | GLY  | 4.9  |
| 25  | YA    | 2164    | C    | 4.9  |
| 22  | QW    | 56      | C    | 4.9  |
| 25  | RA    | 1104    | C    | 4.9  |
| 23  | XX    | 12      | A    | 4.9  |
| 9   | XI    | 23      | ASN  | 4.9  |
| 25  | RA    | 1080    | C    | 4.9  |
| 25  | RA    | 2896    | C    | 4.9  |
| 44  | YY    | 90      | LEU  | 4.9  |
| 55  | R9    | 2       | LYS  | 4.8  |
| 1   | XA    | 1030(B) | C    | 4.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | RA    | 1537 | C    | 4.8  |
| 52  | Y6    | 17   | LYS  | 4.8  |
| 22  | QW    | 49   | G    | 4.8  |
| 25  | YA    | 1176 | G    | 4.8  |
| 55  | Y9    | 12   | ASP  | 4.8  |
| 2   | QB    | 228  | GLY  | 4.8  |
| 44  | YY    | 91   | GLU  | 4.8  |
| 25  | RA    | 2110 | G    | 4.8  |
| 25  | RA    | 2145 | C    | 4.8  |
| 1   | XA    | 202  | U    | 4.8  |
| 30  | YG    | 182  | LYS  | 4.8  |
| 46  | R0    | 7    | LEU  | 4.8  |
| 25  | RA    | 2161 | C    | 4.8  |
| 25  | YA    | 1096 | A    | 4.8  |
| 23  | QX    | 4    | A    | 4.8  |
| 25  | RA    | 2159 | G    | 4.8  |
| 25  | YA    | 2174 | C    | 4.8  |
| 55  | Y9    | 27   | CYS  | 4.7  |
| 25  | YA    | 1092 | C    | 4.7  |
| 25  | YA    | 2158 | A    | 4.7  |
| 23  | XX    | 3    | C    | 4.7  |
| 4   | XD    | 35   | ARG  | 4.7  |
| 22  | QW    | 10   | G    | 4.7  |
| 25  | YA    | 2165 | G    | 4.7  |
| 55  | R9    | 24   | TYR  | 4.7  |
| 25  | RA    | 2124 | G    | 4.7  |
| 45  | RZ    | 152  | ALA  | 4.7  |
| 25  | RA    | 1059 | G    | 4.7  |
| 23  | XX    | 5    | A    | 4.7  |
| 25  | RA    | 2152 | G    | 4.7  |
| 42  | YW    | 113  | LYS  | 4.7  |
| 45  | YZ    | 4    | ARG  | 4.6  |
| 55  | R9    | 9    | ARG  | 4.6  |
| 25  | YA    | 1058 | G    | 4.6  |
| 1   | XA    | 1027 | C    | 4.6  |
| 31  | YH    | 43   | VAL  | 4.6  |
| 55  | R9    | 4    | ARG  | 4.6  |
| 25  | RA    | 1060 | U    | 4.6  |
| 55  | Y9    | 6    | SER  | 4.6  |
| 25  | YA    | 2126 | A    | 4.6  |
| 55  | R9    | 32   | HIS  | 4.5  |
| 22  | XW    | 60   | U    | 4.5  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | QA           | 3          | G           | 4.5         |
| 55         | Y9           | 30         | PRO         | 4.5         |
| 51         | R5           | 59         | GLU         | 4.5         |
| 50         | R4           | 22         | ILE         | 4.5         |
| 32         | YI           | 57         | ARG         | 4.5         |
| 2          | XB           | 232        | PRO         | 4.5         |
| 25         | YA           | 1177       | A           | 4.5         |
| 1          | QA           | 1030(A)    | G           | 4.5         |
| 46         | R0           | 6          | GLY         | 4.5         |
| 25         | RA           | 2115       | G           | 4.5         |
| 11         | QK           | 127        | LYS         | 4.5         |
| 55         | R9           | 17         | ILE         | 4.5         |
| 1          | XA           | 1030(A)    | G           | 4.5         |
| 25         | RA           | 1071       | G           | 4.5         |
| 27         | YD           | 26         | LYS         | 4.5         |
| 25         | RA           | 1058       | G           | 4.4         |
| 31         | RH           | 104        | GLU         | 4.4         |
| 31         | YH           | 3          | ARG         | 4.4         |
| 9          | QI           | 17         | VAL         | 4.4         |
| 25         | RA           | 2120       | G           | 4.4         |
| 25         | YA           | 2104       | G           | 4.4         |
| 24         | QY           | 1          | GLY         | 4.4         |
| 31         | RH           | 3          | ARG         | 4.4         |
| 28         | YE           | 60         | ASN         | 4.4         |
| 55         | R9           | 16         | VAL         | 4.4         |
| 50         | Y4           | 40         | HIS         | 4.4         |
| 25         | RA           | 1535       | U           | 4.4         |
| 25         | RA           | 2122       | U           | 4.3         |
| 25         | RA           | 2897       | U           | 4.3         |
| 23         | QX           | 10         | G           | 4.3         |
| 25         | YA           | 1103       | A           | 4.3         |
| 31         | RH           | 98         | LEU         | 4.3         |
| 23         | QX           | 11         | U           | 4.3         |
| 52         | Y6           | 42         | TRP         | 4.3         |
| 25         | RA           | 2123       | G           | 4.3         |
| 38         | RS           | 111        | GLU         | 4.3         |
| 52         | R6           | 51         | GLU         | 4.3         |
| 25         | YA           | 2794       | C           | 4.3         |
| 31         | YH           | 58         | GLU         | 4.3         |
| 22         | QV           | 47         | U           | 4.3         |
| 25         | YA           | 277        | C           | 4.3         |
| 45         | YZ           | 108        | PRO         | 4.3         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 54  | R8    | 65   | GLU  | 4.3  |
| 9   | QI    | 15   | ALA  | 4.3  |
| 29  | YF    | 133  | ASN  | 4.3  |
| 22  | QW    | 57   | A    | 4.3  |
| 22  | XW    | 72   | A    | 4.3  |
| 3   | QC    | 80   | GLY  | 4.2  |
| 52  | R6    | 40   | CYS  | 4.2  |
| 29  | YF    | 21   | ALA  | 4.2  |
| 25  | YA    | 2122 | U    | 4.2  |
| 1   | QA    | 1004 | A    | 4.2  |
| 22  | QW    | 26   | G    | 4.2  |
| 7   | XG    | 85   | TYR  | 4.2  |
| 31  | YH    | 10   | PRO  | 4.2  |
| 2   | XB    | 16   | HIS  | 4.2  |
| 22  | XW    | 4    | G    | 4.2  |
| 22  | XW    | 52   | G    | 4.2  |
| 25  | YA    | 1085 | A    | 4.2  |
| 22  | QW    | 36   | U    | 4.2  |
| 2   | XB    | 96   | ARG  | 4.2  |
| 52  | Y6    | 45   | LYS  | 4.2  |
| 22  | QW    | 27   | U    | 4.1  |
| 25  | YA    | 1069 | A    | 4.1  |
| 25  | YA    | 2112 | G    | 4.1  |
| 55  | Y9    | 7    | VAL  | 4.1  |
| 25  | YA    | 2894 | G    | 4.1  |
| 22  | XW    | 63   | G    | 4.1  |
| 25  | RA    | 2133 | G    | 4.1  |
| 25  | YA    | 2167 | U    | 4.1  |
| 22  | XW    | 14   | A    | 4.1  |
| 54  | Y8    | 64   | TYR  | 4.1  |
| 22  | QW    | 5    | G    | 4.1  |
| 10  | QJ    | 101  | VAL  | 4.1  |
| 55  | Y9    | 13   | LYS  | 4.1  |
| 10  | QJ    | 34   | VAL  | 4.1  |
| 22  | XW    | 33   | U    | 4.1  |
| 25  | YA    | 1076 | C    | 4.1  |
| 25  | YA    | 2105 | C    | 4.1  |
| 44  | RY    | 46   | LYS  | 4.1  |
| 1   | QA    | 1040 | U    | 4.0  |
| 22  | XW    | 57   | A    | 4.0  |
| 45  | YZ    | 9    | TYR  | 4.0  |
| 50  | Y4    | 13   | ARG  | 4.0  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 55  | Y9    | 19      | ARG  | 4.0  |
| 1   | XA    | 1032    | G    | 4.0  |
| 55  | R9    | 25      | VAL  | 4.0  |
| 22  | QW    | 63      | G    | 4.0  |
| 25  | YA    | 2124    | G    | 4.0  |
| 9   | QI    | 23      | ASN  | 4.0  |
| 25  | RA    | 1073    | A    | 4.0  |
| 21  | QU    | 9       | ARG  | 4.0  |
| 1   | QA    | 1030(B) | C    | 4.0  |
| 14  | XN    | 13      | THR  | 4.0  |
| 2   | QB    | 140     | HIS  | 4.0  |
| 22  | XW    | 53      | G    | 3.9  |
| 25  | RA    | 2114    | A    | 3.9  |
| 25  | YA    | 229     | A    | 3.9  |
| 50  | R4    | 46      | GLN  | 3.9  |
| 21  | QU    | 26      | LYS  | 3.9  |
| 25  | RA    | 1103    | A    | 3.9  |
| 47  | Y1    | 97      | LEU  | 3.9  |
| 24  | XY    | 90      | ASP  | 3.9  |
| 21  | XU    | 5       | ASP  | 3.9  |
| 39  | RT    | 2       | ASN  | 3.9  |
| 45  | RZ    | 154     | ASP  | 3.9  |
| 1   | XA    | 1001(A) | G    | 3.9  |
| 26  | YB    | 1(M)    | A    | 3.9  |
| 47  | R1    | 93      | GLU  | 3.9  |
| 1   | QA    | 1038    | C    | 3.9  |
| 25  | YA    | 2178    | C    | 3.9  |
| 30  | RG    | 26      | GLN  | 3.9  |
| 25  | RA    | 2112    | G    | 3.9  |
| 31  | RH    | 24      | VAL  | 3.9  |
| 9   | QI    | 16      | ARG  | 3.9  |
| 25  | RA    | 1063    | G    | 3.9  |
| 25  | RA    | 271(N)  | U    | 3.9  |
| 25  | YA    | 2143    | C    | 3.9  |
| 2   | QB    | 5       | ILE  | 3.9  |
| 24  | QY    | 59      | ASP  | 3.9  |
| 9   | QI    | 18      | PHE  | 3.8  |
| 52  | R6    | 27      | LYS  | 3.8  |
| 25  | YA    | 2168    | G    | 3.8  |
| 52  | Y6    | 41      | PRO  | 3.8  |
| 55  | R9    | 35      | ARG  | 3.8  |
| 50  | R4    | 36      | CYS  | 3.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 22         | QW           | 66         | C           | 3.8         |
| 39         | YT           | 1          | MET         | 3.8         |
| 52         | R6           | 41         | PRO         | 3.8         |
| 21         | QU           | 2          | GLY         | 3.8         |
| 22         | QW           | 8          | U           | 3.8         |
| 50         | Y4           | 53         | GLU         | 3.8         |
| 7          | XG           | 79         | ARG         | 3.8         |
| 31         | YH           | 6          | ARG         | 3.8         |
| 7          | QG           | 83         | ALA         | 3.8         |
| 29         | YF           | 14         | PRO         | 3.8         |
| 31         | YH           | 170        | ARG         | 3.8         |
| 24         | QY           | 58         | GLY         | 3.8         |
| 55         | Y9           | 33         | LYS         | 3.8         |
| 44         | YY           | 50         | ARG         | 3.8         |
| 50         | R4           | 66         | SER         | 3.8         |
| 52         | Y6           | 13         | CYS         | 3.8         |
| 18         | XR           | 20         | ALA         | 3.8         |
| 2          | QB           | 30         | ARG         | 3.8         |
| 55         | R9           | 19         | ARG         | 3.8         |
| 46         | Y0           | 4          | LYS         | 3.7         |
| 9          | XI           | 5          | TYR         | 3.7         |
| 19         | XS           | 25         | LYS         | 3.7         |
| 25         | YA           | 654(V)     | A           | 3.7         |
| 31         | YH           | 111        | HIS         | 3.7         |
| 1          | XA           | 470        | C           | 3.7         |
| 28         | YE           | 69         | LYS         | 3.7         |
| 55         | R9           | 20         | HIS         | 3.7         |
| 1          | QA           | 1034       | G           | 3.7         |
| 23         | XX           | 10         | G           | 3.7         |
| 25         | RA           | 2146       | C           | 3.7         |
| 14         | QN           | 10         | ALA         | 3.7         |
| 11         | XK           | 129        | SER         | 3.7         |
| 44         | YY           | 88         | LYS         | 3.7         |
| 31         | RH           | 20         | ALA         | 3.7         |
| 22         | QW           | 18         | G           | 3.7         |
| 52         | R6           | 6          | ARG         | 3.7         |
| 22         | QW           | 50         | U           | 3.7         |
| 1          | QA           | 1027       | C           | 3.7         |
| 55         | R9           | 8          | LYS         | 3.7         |
| 3          | QC           | 63         | ASN         | 3.7         |
| 55         | Y9           | 24         | TYR         | 3.7         |
| 2          | QB           | 40         | HIS         | 3.7         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | QS    | 17   | GLU  | 3.7  |
| 25  | RA    | 1061 | U    | 3.7  |
| 44  | RY    | 86   | ARG  | 3.7  |
| 21  | XU    | 26   | LYS  | 3.6  |
| 52  | R6    | 12   | GLU  | 3.6  |
| 22  | QW    | 30   | G    | 3.6  |
| 22  | XW    | 15   | G    | 3.6  |
| 25  | YA    | 2177 | C    | 3.6  |
| 55  | R9    | 3    | VAL  | 3.6  |
| 25  | RA    | 1087 | G    | 3.6  |
| 25  | RA    | 2166 | G    | 3.6  |
| 25  | YA    | 2166 | G    | 3.6  |
| 35  | YP    | 150  | ALA  | 3.6  |
| 25  | RA    | 1052 | C    | 3.6  |
| 25  | RA    | 2129 | C    | 3.6  |
| 45  | RZ    | 9    | TYR  | 3.6  |
| 25  | YA    | 2161 | C    | 3.6  |
| 28  | RE    | 72   | VAL  | 3.6  |
| 52  | R6    | 43   | CYS  | 3.6  |
| 45  | RZ    | 2    | GLU  | 3.6  |
| 29  | RF    | 207  | GLY  | 3.6  |
| 25  | YA    | 1063 | G    | 3.6  |
| 2   | QB    | 41   | ILE  | 3.6  |
| 25  | RA    | 1094 | U    | 3.6  |
| 1   | QA    | 1024 | G    | 3.6  |
| 44  | YY    | 46   | LYS  | 3.6  |
| 53  | Y7    | 48   | LYS  | 3.5  |
| 35  | RP    | 13   | ASN  | 3.5  |
| 46  | Y0    | 85   | ALA  | 3.5  |
| 2   | XB    | 233  | SER  | 3.5  |
| 25  | RA    | 2128 | C    | 3.5  |
| 1   | XA    | 1028 | C    | 3.5  |
| 25  | YA    | 2175 | C    | 3.5  |
| 31  | RH    | 65   | HIS  | 3.5  |
| 25  | RA    | 1111 | A    | 3.5  |
| 55  | Y9    | 22   | ARG  | 3.5  |
| 44  | RY    | 59   | GLY  | 3.5  |
| 25  | RA    | 2158 | A    | 3.5  |
| 25  | RA    | 1105 | U    | 3.5  |
| 1   | QA    | 1535 | C    | 3.5  |
| 7   | QG    | 2    | ALA  | 3.5  |
| 25  | YA    | 1056 | G    | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | RI    | 143  | SER  | 3.5  |
| 25  | YA    | 2142 | C    | 3.5  |
| 24  | XY    | 59   | ASP  | 3.5  |
| 25  | RA    | 1056 | G    | 3.5  |
| 52  | R6    | 36   | LEU  | 3.5  |
| 39  | YT    | 132  | LYS  | 3.5  |
| 1   | XA    | 93   | G    | 3.4  |
| 1   | XA    | 1540 | U    | 3.4  |
| 11  | QK    | 10   | VAL  | 3.4  |
| 22  | XW    | 54   | U    | 3.4  |
| 10  | XJ    | 4    | ILE  | 3.4  |
| 40  | RU    | 91   | ASP  | 3.4  |
| 1   | QA    | 1539 | C    | 3.4  |
| 25  | RA    | 2113 | U    | 3.4  |
| 25  | YA    | 2157 | G    | 3.4  |
| 14  | QN    | 18   | VAL  | 3.4  |
| 22  | QW    | 74   | C    | 3.4  |
| 22  | XW    | 48   | C    | 3.4  |
| 45  | RZ    | 157  | LEU  | 3.4  |
| 1   | QA    | 1537 | U    | 3.4  |
| 50  | Y4    | 63   | TYR  | 3.4  |
| 17  | XQ    | 101  | ARG  | 3.4  |
| 25  | YA    | 2129 | C    | 3.4  |
| 25  | YA    | 2402 | C    | 3.4  |
| 25  | RA    | 1085 | A    | 3.4  |
| 2   | QB    | 131  | PRO  | 3.4  |
| 25  | YA    | 2133 | G    | 3.4  |
| 5   | QE    | 2    | PRO  | 3.4  |
| 25  | YA    | 2150 | U    | 3.4  |
| 32  | YI    | 142  | VAL  | 3.4  |
| 22  | QW    | 61   | C    | 3.4  |
| 25  | YA    | 2893 | G    | 3.4  |
| 50  | R4    | 45   | GLY  | 3.3  |
| 9   | QI    | 64   | THR  | 3.3  |
| 25  | YA    | 2125 | G    | 3.3  |
| 25  | YA    | 2134 | A    | 3.3  |
| 24  | QY    | 7    | HIS  | 3.3  |
| 6   | QF    | 54   | LYS  | 3.3  |
| 25  | RA    | 2793 | G    | 3.3  |
| 14  | XN    | 2    | ALA  | 3.3  |
| 44  | YY    | 102  | CYS  | 3.3  |
| 22  | QW    | 72   | A    | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | RA    | 2137 | C    | 3.3  |
| 21  | QU    | 10   | ARG  | 3.3  |
| 47  | Y1    | 94   | LEU  | 3.3  |
| 14  | QN    | 17   | LYS  | 3.3  |
| 51  | R5    | 60   | VAL  | 3.3  |
| 50  | R4    | 42   | PHE  | 3.3  |
| 21  | QU    | 22   | ARG  | 3.3  |
| 32  | YI    | 85   | GLU  | 3.3  |
| 25  | YA    | 1067 | A    | 3.3  |
| 41  | YV    | 1    | MET  | 3.3  |
| 30  | RG    | 2    | PRO  | 3.2  |
| 21  | XU    | 2    | GLY  | 3.2  |
| 9   | QI    | 88   | TYR  | 3.2  |
| 44  | YY    | 89   | PHE  | 3.2  |
| 13  | XM    | 42   | ALA  | 3.2  |
| 3   | QC    | 193  | TYR  | 3.2  |
| 47  | Y1    | 98   | LEU  | 3.2  |
| 2   | QB    | 136  | VAL  | 3.2  |
| 22  | QW    | 28   | C    | 3.2  |
| 22  | QW    | 67   | C    | 3.2  |
| 25  | YA    | 2896 | C    | 3.2  |
| 55  | R9    | 33   | LYS  | 3.2  |
| 22  | XV    | 47   | U    | 3.2  |
| 25  | RA    | 2140 | C    | 3.2  |
| 23  | XX    | 11   | U    | 3.2  |
| 51  | R5    | 54   | GLY  | 3.2  |
| 25  | YA    | 1098 | A    | 3.2  |
| 25  | YA    | 2135 | A    | 3.2  |
| 31  | RH    | 21   | PRO  | 3.2  |
| 40  | RU    | 90   | VAL  | 3.2  |
| 25  | YA    | 1055 | G    | 3.2  |
| 48  | R2    | 72   | ALA  | 3.2  |
| 11  | QK    | 11   | LYS  | 3.2  |
| 22  | QW    | 73   | A    | 3.2  |
| 25  | YA    | 2128 | C    | 3.2  |
| 2   | XB    | 44   | LEU  | 3.2  |
| 25  | RA    | 2155 | G    | 3.2  |
| 25  | YA    | 2790 | A    | 3.2  |
| 25  | YA    | 2154 | G    | 3.2  |
| 25  | RA    | 2121 | G    | 3.2  |
| 22  | QW    | 32   | C    | 3.1  |
| 22  | XW    | 3    | C    | 3.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 44         | YY           | 47         | LYS         | 3.1         |
| 29         | YF           | 25         | PRO         | 3.1         |
| 25         | YA           | 1762       | A           | 3.1         |
| 24         | XY           | 46         | LEU         | 3.1         |
| 55         | Y9           | 18         | ARG         | 3.1         |
| 22         | QW           | 11         | A           | 3.1         |
| 23         | QX           | 5          | A           | 3.1         |
| 25         | RA           | 1095       | A           | 3.1         |
| 22         | QW           | 9          | G           | 3.1         |
| 22         | XW           | 55         | U           | 3.1         |
| 49         | R3           | 60         | GLU         | 3.1         |
| 50         | R4           | 63         | TYR         | 3.1         |
| 55         | Y9           | 8          | LYS         | 3.1         |
| 22         | QW           | 1          | C           | 3.1         |
| 24         | XY           | 53         | LEU         | 3.1         |
| 21         | QU           | 23         | PRO         | 3.1         |
| 22         | QW           | 4          | G           | 3.1         |
| 25         | YA           | 1042       | G           | 3.1         |
| 25         | YA           | 2802       | G           | 3.1         |
| 55         | Y9           | 2          | LYS         | 3.1         |
| 50         | Y4           | 48         | ARG         | 3.1         |
| 7          | QG           | 85         | TYR         | 3.1         |
| 1          | QA           | 1534       | A           | 3.1         |
| 1          | XA           | 92         | C           | 3.1         |
| 22         | QW           | 39         | C           | 3.1         |
| 24         | QY           | 19         | THR         | 3.1         |
| 25         | YA           | 546        | C           | 3.1         |
| 50         | R4           | 40         | HIS         | 3.1         |
| 52         | R6           | 13         | CYS         | 3.1         |
| 25         | RA           | 2171       | A           | 3.1         |
| 1          | XA           | 78         | G           | 3.1         |
| 24         | QY           | 24         | ALA         | 3.1         |
| 40         | RU           | 118        | GLY         | 3.1         |
| 31         | YH           | 25         | LYS         | 3.1         |
| 55         | Y9           | 31         | LYS         | 3.1         |
| 55         | Y9           | 35         | ARG         | 3.1         |
| 1          | QA           | 1001(A)    | G           | 3.1         |
| 25         | YA           | 11         | G           | 3.1         |
| 31         | YH           | 41         | MET         | 3.1         |
| 1          | XA           | 1030(D)    | A           | 3.1         |
| 25         | RA           | 1079       | C           | 3.1         |
| 25         | YA           | 2139       | C           | 3.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | RZ    | 108  | PRO  | 3.0  |
| 1   | XA    | 1532 | U    | 3.0  |
| 18  | QR    | 38   | GLU  | 3.0  |
| 41  | YV    | 45   | THR  | 3.0  |
| 25  | RA    | 1509 | C    | 3.0  |
| 42  | YW    | 1    | MET  | 3.0  |
| 2   | XB    | 33   | TYR  | 3.0  |
| 41  | RV    | 101  | GLY  | 3.0  |
| 44  | YY    | 55   | TYR  | 3.0  |
| 25  | RA    | 2174 | C    | 3.0  |
| 25  | YA    | 2804 | C    | 3.0  |
| 10  | QJ    | 28   | ARG  | 3.0  |
| 1   | QA    | 1001 | A    | 3.0  |
| 29  | RF    | 1    | MET  | 3.0  |
| 2   | QB    | 35   | GLU  | 3.0  |
| 55  | Y9    | 23   | VAL  | 3.0  |
| 45  | YZ    | 1    | MET  | 3.0  |
| 14  | QN    | 2    | ALA  | 3.0  |
| 50  | R4    | 53   | GLU  | 3.0  |
| 52  | R6    | 45   | LYS  | 3.0  |
| 2   | XB    | 230  | VAL  | 3.0  |
| 25  | RA    | 2117 | A    | 3.0  |
| 25  | RA    | 2805 | G    | 3.0  |
| 25  | YA    | 2121 | G    | 3.0  |
| 31  | YH    | 8    | PRO  | 3.0  |
| 9   | XI    | 128  | ARG  | 3.0  |
| 10  | QJ    | 17   | ASP  | 3.0  |
| 9   | QI    | 33   | PHE  | 3.0  |
| 25  | YA    | 1082 | U    | 3.0  |
| 25  | YA    | 2170 | A    | 3.0  |
| 13  | XM    | 40   | ASN  | 3.0  |
| 9   | XI    | 3    | GLN  | 3.0  |
| 2   | XB    | 43   | ASP  | 3.0  |
| 55  | R9    | 26   | ILE  | 3.0  |
| 2   | QB    | 125  | PRO  | 3.0  |
| 45  | RZ    | 144  | LEU  | 3.0  |
| 13  | XM    | 12   | ASN  | 3.0  |
| 25  | RA    | 229  | A    | 3.0  |
| 25  | YA    | 1088 | A    | 3.0  |
| 25  | RA    | 1055 | G    | 2.9  |
| 51  | Y5    | 49   | CYS  | 2.9  |
| 1   | XA    | 1446 | U    | 2.9  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | QA    | 1538  | C    | 2.9  |
| 22  | XW    | 32    | C    | 2.9  |
| 31  | RH    | 124   | GLU  | 2.9  |
| 4   | QD    | 35    | ARG  | 2.9  |
| 22  | QW    | 31    | G    | 2.9  |
| 45  | YZ    | 160   | GLY  | 2.9  |
| 3   | XC    | 71    | ALA  | 2.9  |
| 52  | R6    | 20    | ASN  | 2.9  |
| 50  | R4    | 34    | GLU  | 2.9  |
| 22  | QW    | 25    | C    | 2.9  |
| 22  | QW    | 40    | C    | 2.9  |
| 10  | QJ    | 89    | ASP  | 2.9  |
| 50  | Y4    | 46    | GLN  | 2.9  |
| 39  | RT    | 135   | ALA  | 2.9  |
| 25  | YA    | 1083  | U    | 2.9  |
| 49  | Y3    | 2     | PRO  | 2.9  |
| 22  | QW    | 53    | G    | 2.9  |
| 22  | QW    | 64    | G    | 2.9  |
| 31  | RH    | 81    | GLU  | 2.9  |
| 10  | XJ    | 59    | SER  | 2.9  |
| 22  | QW    | 17(A) | U    | 2.9  |
| 31  | YH    | 33    | LEU  | 2.9  |
| 2   | XB    | 135   | GLN  | 2.9  |
| 7   | XG    | 8     | GLU  | 2.9  |
| 1   | XA    | 999   | C    | 2.9  |
| 24  | XY    | 71    | ASN  | 2.9  |
| 25  | RA    | 1049  | C    | 2.9  |
| 25  | RA    | 2136  | C    | 2.9  |
| 25  | YA    | 2137  | C    | 2.9  |
| 25  | YA    | 2895  | U    | 2.9  |
| 36  | RQ    | 83    | MET  | 2.9  |
| 25  | RA    | 1051  | G    | 2.9  |
| 13  | XM    | 47    | ASP  | 2.9  |
| 45  | YZ    | 82    | ARG  | 2.9  |
| 50  | Y4    | 68    | ARG  | 2.9  |
| 10  | QJ    | 93    | GLY  | 2.9  |
| 19  | QS    | 44    | MET  | 2.8  |
| 25  | RA    | 2402  | C    | 2.8  |
| 9   | QI    | 8     | GLY  | 2.8  |
| 22  | XW    | 22    | G    | 2.8  |
| 51  | R5    | 58    | LEU  | 2.8  |
| 52  | R6    | 42    | TRP  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 55  | Y9    | 4    | ARG  | 2.8  |
| 22  | QW    | 55   | U    | 2.8  |
| 25  | RA    | 1100 | C    | 2.8  |
| 24  | QY    | 81   | GLY  | 2.8  |
| 44  | YY    | 53   | PRO  | 2.8  |
| 19  | XS    | 28   | LYS  | 2.8  |
| 3   | QC    | 107  | GLN  | 2.8  |
| 32  | RI    | 59   | ALA  | 2.8  |
| 52  | Y6    | 29   | ASN  | 2.8  |
| 38  | YS    | 110  | LEU  | 2.8  |
| 31  | RH    | 128  | PRO  | 2.8  |
| 21  | XU    | 4    | GLY  | 2.8  |
| 41  | YV    | 86   | GLY  | 2.8  |
| 25  | YA    | 1081 | U    | 2.8  |
| 53  | Y7    | 1    | MET  | 2.8  |
| 38  | RS    | 68   | GLN  | 2.8  |
| 31  | RH    | 50   | VAL  | 2.8  |
| 4   | XD    | 145  | GLU  | 2.8  |
| 25  | RA    | 645  | C    | 2.8  |
| 28  | YE    | 76   | ARG  | 2.8  |
| 52  | Y6    | 43   | CYS  | 2.8  |
| 31  | YH    | 4    | ILE  | 2.8  |
| 7   | XG    | 2    | ALA  | 2.8  |
| 47  | R1    | 96   | LYS  | 2.8  |
| 22  | QW    | 52   | G    | 2.8  |
| 23  | XX    | 13   | A    | 2.8  |
| 55  | R9    | 7    | VAL  | 2.8  |
| 35  | YP    | 13   | ASN  | 2.8  |
| 45  | YZ    | 148  | ASP  | 2.8  |
| 25  | YA    | 276  | A    | 2.8  |
| 9   | QI    | 93   | ARG  | 2.8  |
| 9   | QI    | 5    | TYR  | 2.8  |
| 13  | XM    | 41   | PRO  | 2.8  |
| 27  | RD    | 26   | LYS  | 2.8  |
| 31  | YH    | 26   | VAL  | 2.8  |
| 25  | RA    | 1069 | A    | 2.8  |
| 25  | RA    | 2164 | C    | 2.8  |
| 1   | XA    | 1034 | G    | 2.7  |
| 22  | XW    | 45   | G    | 2.7  |
| 25  | RA    | 1177 | A    | 2.7  |
| 25  | YA    | 1048 | A    | 2.7  |
| 39  | RT    | 106  | SER  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | XB    | 37   | ASN  | 2.7  |
| 35  | YP    | 110  | TYR  | 2.7  |
| 52  | Y6    | 40   | CYS  | 2.7  |
| 22  | XW    | 70   | G    | 2.7  |
| 19  | QS    | 21   | GLU  | 2.7  |
| 1   | QA    | 1138 | G    | 2.7  |
| 9   | XI    | 20   | ARG  | 2.7  |
| 3   | QC    | 105  | GLU  | 2.7  |
| 9   | XI    | 126  | SER  | 2.7  |
| 55  | R9    | 18   | ARG  | 2.7  |
| 52  | Y6    | 14   | THR  | 2.7  |
| 25  | RA    | 1048 | A    | 2.7  |
| 25  | RA    | 2170 | A    | 2.7  |
| 25  | RA    | 2190 | G    | 2.7  |
| 2   | QB    | 21   | ARG  | 2.7  |
| 12  | XL    | 126  | LYS  | 2.7  |
| 31  | RH    | 58   | GLU  | 2.7  |
| 28  | RE    | 50   | GLY  | 2.7  |
| 50  | Y4    | 70   | GLY  | 2.7  |
| 51  | Y5    | 2    | ALA  | 2.7  |
| 22  | QW    | 22   | G    | 2.7  |
| 25  | YA    | 2162 | G    | 2.7  |
| 1   | XA    | 1541 | U    | 2.7  |
| 10  | XJ    | 78   | ASN  | 2.7  |
| 20  | QT    | 9    | ASN  | 2.7  |
| 25  | RA    | 2105 | C    | 2.7  |
| 25  | YA    | 2189 | U    | 2.7  |
| 5   | XE    | 155  | GLU  | 2.7  |
| 7   | QG    | 5    | ARG  | 2.7  |
| 19  | XS    | 43   | GLU  | 2.7  |
| 52  | Y6    | 30   | THR  | 2.7  |
| 2   | QB    | 135  | GLN  | 2.7  |
| 31  | RH    | 48   | GLY  | 2.7  |
| 25  | YA    | 2109 | U    | 2.7  |
| 1   | QA    | 1533 | C    | 2.7  |
| 3   | QC    | 146  | ALA  | 2.7  |
| 31  | YH    | 104  | GLU  | 2.7  |
| 55  | Y9    | 26   | ILE  | 2.7  |
| 24  | XY    | 35   | GLN  | 2.7  |
| 4   | XD    | 12   | CYS  | 2.7  |
| 25  | YA    | 2144 | U    | 2.7  |
| 29  | YF    | 7    | TYR  | 2.7  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | XA           | 630        | G           | 2.7         |
| 22         | QW           | 65         | C           | 2.7         |
| 24         | QY           | 46         | LEU         | 2.7         |
| 25         | YA           | 1041       | C           | 2.7         |
| 17         | QQ           | 2          | PRO         | 2.7         |
| 31         | YH           | 46         | GLU         | 2.7         |
| 29         | RF           | 128        | ALA         | 2.7         |
| 27         | RD           | 99         | ASP         | 2.7         |
| 50         | Y4           | 52         | THR         | 2.7         |
| 25         | RA           | 1092       | C           | 2.7         |
| 48         | Y2           | 43         | GLN         | 2.7         |
| 23         | XX           | 9          | G           | 2.7         |
| 25         | YA           | 1089       | G           | 2.7         |
| 50         | R4           | 64         | GLY         | 2.7         |
| 55         | R9           | 30         | PRO         | 2.7         |
| 25         | YA           | 2897       | U           | 2.6         |
| 31         | RH           | 10         | PRO         | 2.6         |
| 19         | QS           | 38         | SER         | 2.6         |
| 45         | YZ           | 135        | GLU         | 2.6         |
| 47         | Y1           | 93         | GLU         | 2.6         |
| 23         | QX           | 13         | A           | 2.6         |
| 9          | XI           | 6          | GLY         | 2.6         |
| 1          | XA           | 1542       | U           | 2.6         |
| 6          | QF           | 101        | ALA         | 2.6         |
| 10         | QJ           | 85         | LEU         | 2.6         |
| 11         | QK           | 14         | VAL         | 2.6         |
| 31         | RH           | 23         | ARG         | 2.6         |
| 52         | Y6           | 50         | ARG         | 2.6         |
| 46         | R0           | 3          | HIS         | 2.6         |
| 21         | XU           | 10         | ARG         | 2.6         |
| 24         | QY           | 18         | VAL         | 2.6         |
| 25         | YA           | 1046       | A           | 2.6         |
| 25         | YA           | 1077       | A           | 2.6         |
| 10         | QJ           | 67         | THR         | 2.6         |
| 7          | XG           | 5          | ARG         | 2.6         |
| 2          | QB           | 132        | LYS         | 2.6         |
| 10         | QJ           | 54         | PHE         | 2.6         |
| 1          | QA           | 1087       | G           | 2.6         |
| 22         | QW           | 15         | G           | 2.6         |
| 22         | XW           | 9          | G           | 2.6         |
| 22         | XW           | 49         | G           | 2.6         |
| 25         | YA           | 2152       | G           | 2.6         |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 38  | YS    | 2     | ALA  | 2.6  |
| 2   | QB    | 232   | PRO  | 2.6  |
| 41  | RV    | 45    | THR  | 2.6  |
| 6   | QF    | 59    | TYR  | 2.6  |
| 31  | YH    | 137   | ASP  | 2.6  |
| 36  | YQ    | 91    | GLU  | 2.6  |
| 25  | RA    | 1110  | G    | 2.6  |
| 25  | RA    | 888   | C    | 2.6  |
| 25  | RA    | 2188  | C    | 2.6  |
| 25  | RA    | 2506  | U    | 2.6  |
| 23  | XX    | 6     | G    | 2.6  |
| 1   | QA    | 1039  | C    | 2.6  |
| 10  | QJ    | 27    | ALA  | 2.6  |
| 22  | QW    | 41    | C    | 2.6  |
| 22  | XW    | 17(A) | U    | 2.6  |
| 25  | YA    | 2136  | C    | 2.6  |
| 31  | YH    | 54    | ARG  | 2.6  |
| 14  | XN    | 10    | ALA  | 2.5  |
| 22  | XW    | 64    | G    | 2.5  |
| 23  | QX    | 6     | G    | 2.5  |
| 25  | RA    | 2104  | G    | 2.5  |
| 25  | RA    | 2147  | G    | 2.5  |
| 25  | RA    | 1098  | A    | 2.5  |
| 1   | QA    | 1002  | G    | 2.5  |
| 22  | XW    | 31    | G    | 2.5  |
| 31  | RH    | 115   | VAL  | 2.5  |
| 36  | RQ    | 27    | VAL  | 2.5  |
| 1   | XA    | 1533  | C    | 2.5  |
| 22  | XW    | 71    | C    | 2.5  |
| 9   | XI    | 125   | TYR  | 2.5  |
| 25  | RA    | 2792  | G    | 2.5  |
| 35  | YP    | 65    | ARG  | 2.5  |
| 10  | QJ    | 24    | VAL  | 2.5  |
| 22  | XW    | 21    | A    | 2.5  |
| 31  | YH    | 45    | VAL  | 2.5  |
| 39  | YT    | 136   | GLN  | 2.5  |
| 55  | Y9    | 21    | GLY  | 2.5  |
| 55  | Y9    | 37    | GLY  | 2.5  |
| 9   | XI    | 18    | PHE  | 2.5  |
| 52  | R6    | 37    | ARG  | 2.5  |
| 10  | XJ    | 35    | SER  | 2.5  |
| 25  | RA    | 2130  | U    | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 31  | RH    | 27   | LYS  | 2.5  |
| 44  | RY    | 45   | VAL  | 2.5  |
| 9   | QI    | 128  | ARG  | 2.5  |
| 22  | QW    | 71   | C    | 2.5  |
| 25  | RA    | 1086 | A    | 2.5  |
| 1   | XA    | 1024 | G    | 2.5  |
| 25  | YA    | 2793 | G    | 2.5  |
| 35  | RP    | 65   | ARG  | 2.5  |
| 14  | QN    | 61   | TRP  | 2.5  |
| 31  | YH    | 72   | ILE  | 2.5  |
| 50  | R4    | 24   | THR  | 2.5  |
| 2   | QB    | 9    | GLU  | 2.5  |
| 29  | YF    | 2    | LYS  | 2.5  |
| 22  | XW    | 11   | A    | 2.5  |
| 13  | QM    | 57   | ARG  | 2.5  |
| 52  | Y6    | 53   | LYS  | 2.5  |
| 29  | YF    | 18   | ARG  | 2.5  |
| 3   | XC    | 73   | PRO  | 2.5  |
| 22  | XW    | 17   | C    | 2.5  |
| 51  | Y5    | 53   | ALA  | 2.5  |
| 22  | XW    | 59   | A    | 2.5  |
| 21  | QU    | 14   | TRP  | 2.5  |
| 1   | QA    | 1159 | U    | 2.5  |
| 9   | QI    | 92   | TYR  | 2.5  |
| 31  | YH    | 99   | VAL  | 2.5  |
| 32  | RI    | 115  | ALA  | 2.5  |
| 45  | YZ    | 77   | ASP  | 2.5  |
| 1   | QA    | 1536 | C    | 2.5  |
| 52  | Y6    | 44   | ARG  | 2.5  |
| 22  | QW    | 20   | U    | 2.5  |
| 20  | XT    | 106  | ALA  | 2.5  |
| 2   | QB    | 111  | ARG  | 2.5  |
| 31  | YH    | 9    | ILE  | 2.5  |
| 45  | RZ    | 151  | HIS  | 2.5  |
| 52  | Y6    | 12   | GLU  | 2.5  |
| 55  | R9    | 10   | ILE  | 2.5  |
| 22  | QW    | 69   | C    | 2.4  |
| 25  | YA    | 1509 | C    | 2.4  |
| 25  | YA    | 2140 | C    | 2.4  |
| 2   | QB    | 7    | VAL  | 2.4  |
| 32  | RI    | 58   | LEU  | 2.4  |
| 46  | R0    | 5    | LYS  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | XB    | 5    | ILE  | 2.4  |
| 31  | YH    | 57   | ASP  | 2.4  |
| 33  | YN    | 130  | HIS  | 2.4  |
| 1   | QA    | 1029 | C    | 2.4  |
| 23  | QX    | 9    | G    | 2.4  |
| 25  | RA    | 2131 | G    | 2.4  |
| 25  | RA    | 2154 | G    | 2.4  |
| 51  | R5    | 2    | ALA  | 2.4  |
| 13  | XM    | 117  | VAL  | 2.4  |
| 32  | YI    | 75   | LEU  | 2.4  |
| 39  | RT    | 6    | LEU  | 2.4  |
| 1   | QA    | 1532 | U    | 2.4  |
| 22  | XW    | 12   | G    | 2.4  |
| 23  | QX    | 22   | U    | 2.4  |
| 25  | YA    | 2147 | G    | 2.4  |
| 7   | QG    | 9    | VAL  | 2.4  |
| 55  | R9    | 5    | ALA  | 2.4  |
| 32  | RI    | 125  | GLU  | 2.4  |
| 13  | XM    | 102  | ARG  | 2.4  |
| 43  | RX    | 70   | LEU  | 2.4  |
| 1   | QA    | 1142 | G    | 2.4  |
| 50  | R4    | 17   | GLY  | 2.4  |
| 55  | R9    | 37   | GLY  | 2.4  |
| 12  | XL    | 128  | ALA  | 2.4  |
| 18  | QR    | 19   | LYS  | 2.4  |
| 50  | R4    | 12   | ALA  | 2.4  |
| 36  | RQ    | 91   | GLU  | 2.4  |
| 54  | Y8    | 56   | GLU  | 2.4  |
| 2   | XB    | 48   | MET  | 2.4  |
| 7   | QG    | 73   | MET  | 2.4  |
| 10  | QJ    | 90   | LEU  | 2.4  |
| 45  | RZ    | 107  | THR  | 2.4  |
| 1   | XA    | 1534 | A    | 2.4  |
| 7   | QG    | 156  | TRP  | 2.4  |
| 22  | XW    | 19   | G    | 2.4  |
| 25  | YA    | 2792 | G    | 2.4  |
| 3   | XC    | 85   | ARG  | 2.4  |
| 44  | RY    | 60   | PHE  | 2.4  |
| 52  | R6    | 53   | LYS  | 2.4  |
| 7   | XG    | 153  | HIS  | 2.4  |
| 44  | RY    | 99   | CYS  | 2.4  |
| 2   | QB    | 240  | GLN  | 2.4  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 3   | XC    | 86      | VAL  | 2.4  |
| 3   | XC    | 178     | LEU  | 2.4  |
| 3   | XC    | 192     | THR  | 2.4  |
| 20  | QT    | 99      | LEU  | 2.4  |
| 25  | RA    | 897     | C    | 2.4  |
| 1   | XA    | 1004    | A    | 2.4  |
| 23  | QX    | 8       | A    | 2.4  |
| 3   | QC    | 191     | THR  | 2.4  |
| 21  | QU    | 17      | THR  | 2.4  |
| 38  | RS    | 2       | ALA  | 2.4  |
| 9   | QI    | 63      | ILE  | 2.4  |
| 1   | XA    | 1442(B) | A    | 2.4  |
| 14  | QN    | 13      | THR  | 2.4  |
| 51  | R5    | 53      | ALA  | 2.4  |
| 54  | R8    | 34      | TRP  | 2.4  |
| 1   | QA    | 1136    | U    | 2.4  |
| 3   | XC    | 82      | GLU  | 2.4  |
| 25  | RA    | 2179    | C    | 2.4  |
| 19  | QS    | 36      | ARG  | 2.3  |
| 9   | QI    | 126     | SER  | 2.3  |
| 25  | RA    | 1091    | G    | 2.3  |
| 25  | YA    | 2148    | G    | 2.3  |
| 25  | YA    | 2153    | G    | 2.3  |
| 7   | XG    | 155     | ARG  | 2.3  |
| 44  | YY    | 86      | ARG  | 2.3  |
| 1   | QA    | 1286    | A    | 2.3  |
| 22  | QW    | 37      | A    | 2.3  |
| 50  | Y4    | 60      | GLN  | 2.3  |
| 1   | XA    | 1036    | G    | 2.3  |
| 4   | QD    | 12      | CYS  | 2.3  |
| 25  | RA    | 2807    | G    | 2.3  |
| 9   | XI    | 2       | GLU  | 2.3  |
| 22  | XW    | 74      | C    | 2.3  |
| 24  | XY    | 25      | GLN  | 2.3  |
| 28  | RE    | 77      | ILE  | 2.3  |
| 39  | YT    | 130     | ALA  | 2.3  |
| 9   | XI    | 26      | VAL  | 2.3  |
| 50  | R4    | 69      | LYS  | 2.3  |
| 51  | Y5    | 3       | LYS  | 2.3  |
| 25  | RA    | 1044    | G    | 2.3  |
| 39  | RT    | 129     | ARG  | 2.3  |
| 3   | QC    | 27      | LYS  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | QW    | 44   | A    | 2.3  |
| 31  | YH    | 103  | LEU  | 2.3  |
| 55  | Y9    | 5    | ALA  | 2.3  |
| 22  | XW    | 30   | G    | 2.3  |
| 22  | XW    | 50   | U    | 2.3  |
| 31  | RH    | 51   | ARG  | 2.3  |
| 32  | RI    | 135  | GLU  | 2.3  |
| 2   | QB    | 118  | LEU  | 2.3  |
| 55  | R9    | 15   | LYS  | 2.3  |
| 50  | R4    | 65   | ASP  | 2.3  |
| 38  | RS    | 46   | VAL  | 2.3  |
| 4   | XD    | 47   | ARG  | 2.3  |
| 29  | RF    | 14   | PRO  | 2.3  |
| 31  | RH    | 42   | ARG  | 2.3  |
| 31  | RH    | 130  | ARG  | 2.3  |
| 22  | QW    | 45   | G    | 2.3  |
| 25  | RA    | 2106 | G    | 2.3  |
| 25  | YA    | 2102 | U    | 2.3  |
| 24  | XY    | 39   | THR  | 2.3  |
| 25  | RA    | 2476 | A    | 2.3  |
| 31  | YH    | 140  | LYS  | 2.3  |
| 25  | RA    | 1053 | C    | 2.3  |
| 24  | QY    | 40   | ALA  | 2.3  |
| 25  | YA    | 2130 | U    | 2.3  |
| 27  | RD    | 268  | ARG  | 2.3  |
| 13  | QM    | 8    | GLU  | 2.3  |
| 25  | YA    | 275  | G    | 2.3  |
| 19  | QS    | 59   | PRO  | 2.3  |
| 52  | R6    | 7    | ILE  | 2.3  |
| 24  | XY    | 9    | GLY  | 2.3  |
| 25  | YA    | 2506 | U    | 2.3  |
| 29  | RF    | 133  | ASN  | 2.3  |
| 38  | RS    | 108  | GLY  | 2.3  |
| 13  | QM    | 47   | ASP  | 2.3  |
| 31  | RH    | 116  | GLU  | 2.3  |
| 31  | YH    | 116  | GLU  | 2.3  |
| 25  | RA    | 1176 | G    | 2.3  |
| 19  | QS    | 25   | LYS  | 2.3  |
| 45  | RZ    | 174  | VAL  | 2.3  |
| 3   | QC    | 194  | GLY  | 2.3  |
| 7   | XG    | 129  | GLU  | 2.3  |
| 1   | XA    | 1006 | C    | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | XJ    | 6    | ILE  | 2.3  |
| 24  | XY    | 18   | VAL  | 2.3  |
| 22  | QW    | 70   | G    | 2.2  |
| 1   | XA    | 841  | U    | 2.2  |
| 24  | QY    | 41   | THR  | 2.2  |
| 39  | RT    | 1    | MET  | 2.2  |
| 52  | Y6    | 37   | ARG  | 2.2  |
| 25  | RA    | 893  | C    | 2.2  |
| 25  | RA    | 1102 | C    | 2.2  |
| 31  | YH    | 136  | ILE  | 2.2  |
| 31  | YH    | 113  | VAL  | 2.2  |
| 1   | QA    | 1035 | A    | 2.2  |
| 24  | QY    | 48   | ARG  | 2.2  |
| 42  | YW    | 92   | ARG  | 2.2  |
| 1   | XA    | 998  | G    | 2.2  |
| 5   | XE    | 5    | ASP  | 2.2  |
| 5   | XE    | 73   | ASN  | 2.2  |
| 22  | XW    | 10   | G    | 2.2  |
| 24  | XY    | 26   | ASP  | 2.2  |
| 2   | XB    | 234  | PRO  | 2.2  |
| 1   | QA    | 1019 | C    | 2.2  |
| 3   | QC    | 205  | GLY  | 2.2  |
| 6   | QF    | 63   | TYR  | 2.2  |
| 45  | YZ    | 179  | ASP  | 2.2  |
| 2   | QB    | 36   | ARG  | 2.2  |
| 21  | QU    | 11   | GLY  | 2.2  |
| 25  | RA    | 2177 | C    | 2.2  |
| 31  | RH    | 123  | PHE  | 2.2  |
| 9   | QI    | 65   | VAL  | 2.2  |
| 20  | XT    | 98   | PRO  | 2.2  |
| 23  | QX    | 14   | A    | 2.2  |
| 39  | YT    | 131  | ALA  | 2.2  |
| 22  | QW    | 54   | U    | 2.2  |
| 25  | RA    | 2118 | U    | 2.2  |
| 31  | YH    | 65   | HIS  | 2.2  |
| 1   | QA    | 1042 | G    | 2.2  |
| 24  | XY    | 4    | SER  | 2.2  |
| 1   | XA    | 1043 | C    | 2.2  |
| 25  | YA    | 2107 | C    | 2.2  |
| 2   | QB    | 128  | GLU  | 2.2  |
| 24  | XY    | 57   | LYS  | 2.2  |
| 4   | XD    | 26   | CYS  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | XW    | 24   | U    | 2.2  |
| 23  | QX    | 12   | A    | 2.2  |
| 44  | YY    | 99   | CYS  | 2.2  |
| 18  | QR    | 88   | LYS  | 2.2  |
| 19  | XS    | 35   | SER  | 2.2  |
| 21  | QU    | 25   | LYS  | 2.2  |
| 31  | YH    | 110  | SER  | 2.2  |
| 49  | R3    | 3    | ARG  | 2.2  |
| 16  | QP    | 83   | GLU  | 2.2  |
| 23  | QX    | 7    | G    | 2.2  |
| 25  | RA    | 11   | G    | 2.2  |
| 25  | RA    | 1534 | G    | 2.2  |
| 25  | YA    | 2106 | G    | 2.2  |
| 50  | Y4    | 67   | TYR  | 2.2  |
| 2   | XB    | 10   | LEU  | 2.2  |
| 27  | RD    | 262  | ARG  | 2.2  |
| 47  | Y1    | 26   | ARG  | 2.2  |
| 2   | XB    | 134  | GLU  | 2.2  |
| 44  | RY    | 103  | GLY  | 2.2  |
| 52  | R6    | 24   | GLU  | 2.2  |
| 32  | RI    | 137  | PRO  | 2.2  |
| 7   | QG    | 114  | ARG  | 2.2  |
| 25  | RA    | 2833 | G    | 2.2  |
| 39  | YT    | 35   | LYS  | 2.2  |
| 45  | YZ    | 107  | THR  | 2.2  |
| 24  | QY    | 89   | GLU  | 2.2  |
| 50  | R4    | 35   | VAL  | 2.2  |
| 50  | Y4    | 34   | GLU  | 2.2  |
| 52  | R6    | 52   | VAL  | 2.2  |
| 18  | QR    | 77   | GLY  | 2.2  |
| 42  | YW    | 112  | GLY  | 2.2  |
| 25  | RA    | 2134 | A    | 2.2  |
| 2   | XB    | 11   | LEU  | 2.2  |
| 8   | QH    | 102  | ARG  | 2.2  |
| 14  | QN    | 14   | PRO  | 2.2  |
| 45  | RZ    | 140  | ASP  | 2.2  |
| 24  | XY    | 37   | ILE  | 2.2  |
| 10  | QJ    | 70   | ARG  | 2.2  |
| 19  | QS    | 50   | ALA  | 2.2  |
| 25  | YA    | 1097 | U    | 2.2  |
| 4   | XD    | 45   | GLN  | 2.2  |
| 31  | RH    | 109  | PHE  | 2.2  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 36  | YQ    | 61      | GLY  | 2.2  |
| 28  | YE    | 67      | PHE  | 2.2  |
| 26  | RB    | 1(M)    | A    | 2.2  |
| 31  | YH    | 124     | GLU  | 2.2  |
| 40  | YU    | 91      | ASP  | 2.2  |
| 55  | R9    | 23      | VAL  | 2.2  |
| 1   | XA    | 994     | A    | 2.2  |
| 2   | XB    | 21      | ARG  | 2.2  |
| 25  | RA    | 277     | C    | 2.1  |
| 50  | Y4    | 42      | PHE  | 2.1  |
| 25  | RA    | 2189    | U    | 2.1  |
| 31  | RH    | 11      | VAL  | 2.1  |
| 36  | RQ    | 138     | ASP  | 2.1  |
| 44  | RY    | 61      | ILE  | 2.1  |
| 55  | Y9    | 16      | VAL  | 2.1  |
| 2   | QB    | 139     | LYS  | 2.1  |
| 14  | XN    | 11      | LYS  | 2.1  |
| 1   | QA    | 1030(C) | G    | 2.1  |
| 25  | RA    | 2894    | G    | 2.1  |
| 25  | YA    | 653     | A    | 2.1  |
| 38  | RS    | 51      | ALA  | 2.1  |
| 7   | QG    | 78      | ARG  | 2.1  |
| 20  | XT    | 101     | GLY  | 2.1  |
| 22  | XW    | 8       | U    | 2.1  |
| 13  | QM    | 96      | LEU  | 2.1  |
| 20  | XT    | 9       | ASN  | 2.1  |
| 21  | QU    | 8       | THR  | 2.1  |
| 1   | QA    | 630     | G    | 2.1  |
| 2   | XB    | 122     | PHE  | 2.1  |
| 1   | QA    | 1146    | A    | 2.1  |
| 3   | XC    | 179     | ARG  | 2.1  |
| 5   | QE    | 3       | GLU  | 2.1  |
| 9   | QI    | 31      | GLN  | 2.1  |
| 25  | RA    | 2180    | U    | 2.1  |
| 30  | RG    | 97      | ASP  | 2.1  |
| 9   | QI    | 111     | ARG  | 2.1  |
| 24  | XY    | 73      | ARG  | 2.1  |
| 52  | Y6    | 47      | THR  | 2.1  |
| 3   | QC    | 104     | GLN  | 2.1  |
| 10  | QJ    | 23      | ILE  | 2.1  |
| 31  | RH    | 26      | VAL  | 2.1  |
| 10  | QJ    | 10      | GLY  | 2.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 10         | QJ           | 39         | PRO         | 2.1         |
| 22         | XW           | 26         | G           | 2.1         |
| 25         | RA           | 654(O)     | G           | 2.1         |
| 3          | XC           | 149        | ALA         | 2.1         |
| 7          | XG           | 154        | TYR         | 2.1         |
| 10         | QJ           | 99         | LYS         | 2.1         |
| 25         | RA           | 895        | U           | 2.1         |
| 45         | RZ           | 156        | LYS         | 2.1         |
| 30         | YG           | 29         | TRP         | 2.1         |
| 11         | XK           | 117        | ASN         | 2.1         |
| 47         | Y1           | 27         | GLU         | 2.1         |
| 30         | YG           | 52         | ILE         | 2.1         |
| 50         | Y4           | 15         | ILE         | 2.1         |
| 41         | RV           | 36         | PRO         | 2.1         |
| 52         | Y6           | 36         | LEU         | 2.1         |
| 1          | QA           | 1030(D)    | A           | 2.1         |
| 22         | QW           | 29         | G           | 2.1         |
| 25         | RA           | 1047       | G           | 2.1         |
| 21         | XU           | 14         | TRP         | 2.1         |
| 22         | QW           | 23         | C           | 2.1         |
| 25         | YA           | 1104       | C           | 2.1         |
| 52         | Y6           | 32         | ASN         | 2.1         |
| 7          | QG           | 72         | ARG         | 2.1         |
| 2          | QB           | 122        | PHE         | 2.1         |
| 11         | QK           | 43         | SER         | 2.1         |
| 17         | QQ           | 58         | GLU         | 2.1         |
| 50         | Y4           | 56         | VAL         | 2.1         |
| 25         | RA           | 2382       | G           | 2.1         |
| 2          | XB           | 123        | ALA         | 2.1         |
| 24         | QY           | 90         | ASP         | 2.1         |
| 43         | YX           | 3          | THR         | 2.1         |
| 1          | QA           | 1320       | C           | 2.1         |
| 25         | YA           | 883        | G           | 2.1         |
| 25         | YA           | 1072       | C           | 2.1         |
| 25         | YA           | 2891       | G           | 2.1         |
| 10         | XJ           | 98         | ILE         | 2.1         |
| 21         | XU           | 9          | ARG         | 2.1         |
| 30         | RG           | 74         | LYS         | 2.1         |
| 31         | RH           | 134        | SER         | 2.1         |
| 50         | R4           | 39         | CYS         | 2.1         |
| 31         | YH           | 82         | GLY         | 2.1         |
| 31         | RH           | 129        | THR         | 2.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 24  | XY    | 69   | ARG  | 2.1  |
| 39  | YT    | 3    | ARG  | 2.1  |
| 45  | YZ    | 80   | ARG  | 2.1  |
| 52  | R6    | 17   | LYS  | 2.1  |
| 1   | XA    | 1029 | C    | 2.1  |
| 31  | YH    | 49   | VAL  | 2.1  |
| 1   | QA    | 1182 | G    | 2.1  |
| 3   | XC    | 72   | LYS  | 2.1  |
| 3   | QC    | 192  | THR  | 2.1  |
| 35  | YP    | 149  | GLU  | 2.1  |
| 3   | QC    | 204  | LEU  | 2.1  |
| 2   | XB    | 9    | GLU  | 2.0  |
| 9   | QI    | 4    | TYR  | 2.0  |
| 25  | RA    | 1062 | G    | 2.0  |
| 19  | QS    | 53   | ASN  | 2.0  |
| 31  | RH    | 102  | ALA  | 2.0  |
| 25  | RA    | 1026 | U    | 2.0  |
| 25  | RA    | 2144 | U    | 2.0  |
| 31  | YH    | 68   | THR  | 2.0  |
| 22  | XW    | 76   | A    | 2.0  |
| 25  | RA    | 1084 | A    | 2.0  |
| 30  | RG    | 182  | LYS  | 2.0  |
| 24  | XY    | 70   | ALA  | 2.0  |
| 45  | YZ    | 86   | VAL  | 2.0  |
| 22  | QW    | 12   | G    | 2.0  |
| 25  | RA    | 100  | G    | 2.0  |
| 10  | XJ    | 79   | ARG  | 2.0  |
| 35  | YP    | 16   | ARG  | 2.0  |
| 44  | RY    | 2    | ARG  | 2.0  |
| 19  | QS    | 4    | SER  | 2.0  |
| 31  | YH    | 32   | GLU  | 2.0  |
| 1   | XA    | 1531 | A    | 2.0  |
| 32  | YI    | 141  | LYS  | 2.0  |
| 22  | XW    | 37   | A    | 2.0  |
| 4   | QD    | 26   | CYS  | 2.0  |
| 9   | QI    | 3    | GLN  | 2.0  |
| 11  | QK    | 80   | VAL  | 2.0  |
| 13  | QM    | 45   | VAL  | 2.0  |
| 40  | YU    | 92   | ARG  | 2.0  |
| 1   | QA    | 1032 | G    | 2.0  |
| 3   | XC    | 81   | GLY  | 2.0  |
| 7   | QG    | 8    | GLU  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 23  | A2M  | QX    | 19  | 23/24 | 0.85 | 0.36 | -    | 108,108,108,108            | 0     |
| 23  | A2M  | XX    | 20  | 23/24 | 0.90 | 0.25 | -    | 107,107,108,108            | 0     |
| 23  | A2M  | QX    | 21  | 23/24 | 0.84 | 0.31 | -    | 108,155,155,155            | 0     |
| 23  | A2M  | QX    | 20  | 23/24 | 0.90 | 0.26 | -    | 108,114,114,114            | 0     |
| 23  | A2M  | XX    | 21  | 23/24 | 0.84 | 0.30 | -    | 108,164,164,164            | 0     |
| 23  | A2M  | XX    | 19  | 23/24 | 0.88 | 0.26 | -    | 99,99,108,108              | 0     |

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 56  | MG   | RA    | 3244 | 1/1   | 0.89 | 0.46 | 64.82 | 16,16,16,16                | 0     |
| 56  | MG   | RA    | 3263 | 1/1   | 0.88 | 0.81 | 62.70 | 31,31,31,31                | 0     |
| 56  | MG   | YA    | 3080 | 1/1   | 0.94 | 0.49 | 48.60 | 15,15,15,15                | 0     |
| 56  | MG   | RA    | 3063 | 1/1   | 0.98 | 0.63 | 47.99 | 29,29,29,29                | 0     |
| 56  | MG   | YA    | 3049 | 1/1   | 0.99 | 0.47 | 46.52 | 12,12,12,12                | 0     |
| 56  | MG   | YA    | 3375 | 1/1   | 0.91 | 0.52 | 41.60 | 51,51,51,51                | 0     |
| 56  | MG   | RA    | 3275 | 1/1   | 0.87 | 0.83 | 39.18 | 48,48,48,48                | 0     |
| 56  | MG   | RA    | 3411 | 1/1   | 0.84 | 0.82 | 39.08 | 29,29,29,29                | 0     |
| 56  | MG   | YA    | 3054 | 1/1   | 0.98 | 0.48 | 38.85 | 1,1,1,1                    | 0     |
| 56  | MG   | RA    | 3165 | 1/1   | 0.92 | 0.55 | 36.19 | 25,25,25,25                | 0     |
| 56  | MG   | XA    | 1652 | 1/1   | 0.93 | 0.73 | 33.96 | 48,48,48,48                | 0     |
| 56  | MG   | RA    | 3363 | 1/1   | 0.95 | 0.65 | 33.27 | 34,34,34,34                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | YA    | 3335 | 1/1   | 0.95 | 0.50 | 32.82 | 16,16,16,16                 | 0     |
| 56  | MG   | YA    | 3025 | 1/1   | 0.98 | 0.63 | 31.54 | 16,16,16,16                 | 0     |
| 56  | MG   | YA    | 3280 | 1/1   | 0.90 | 0.73 | 30.79 | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1640 | 1/1   | 0.99 | 0.38 | 30.48 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3002 | 1/1   | 0.79 | 0.63 | 29.98 | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3472 | 1/1   | 0.78 | 0.54 | 29.52 | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3190 | 1/1   | 0.91 | 0.74 | 29.30 | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3081 | 1/1   | 0.98 | 0.49 | 28.76 | 7,7,7,7                     | 0     |
| 56  | MG   | RA    | 3292 | 1/1   | 0.95 | 0.71 | 28.72 | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3295 | 1/1   | 0.91 | 0.39 | 28.53 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3079 | 1/1   | 0.98 | 0.47 | 27.59 | 10,10,10,10                 | 0     |
| 56  | MG   | RA    | 3331 | 1/1   | 0.78 | 0.32 | 27.17 | 69,69,69,69                 | 0     |
| 56  | MG   | RA    | 3012 | 1/1   | 0.96 | 0.76 | 26.88 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3460 | 1/1   | 0.89 | 0.61 | 26.63 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3081 | 1/1   | 0.97 | 0.34 | 26.54 | 4,4,4,4                     | 0     |
| 56  | MG   | RA    | 3369 | 1/1   | 0.96 | 0.54 | 25.84 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3325 | 1/1   | 0.98 | 0.37 | 25.28 | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3192 | 1/1   | 0.84 | 0.64 | 24.84 | 23,23,23,23                 | 0     |
| 56  | MG   | RA    | 3055 | 1/1   | 0.97 | 0.51 | 24.33 | 10,10,10,10                 | 0     |
| 56  | MG   | YA    | 3455 | 1/1   | 0.94 | 0.47 | 23.91 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3173 | 1/1   | 0.99 | 0.44 | 23.58 | 5,5,5,5                     | 0     |
| 56  | MG   | RA    | 3082 | 1/1   | 0.99 | 0.45 | 23.48 | 0,0,0,0                     | 0     |
| 56  | MG   | XA    | 1701 | 1/1   | 0.96 | 0.34 | 23.45 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3195 | 1/1   | 0.98 | 0.61 | 23.16 | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3189 | 1/1   | 0.98 | 0.46 | 22.85 | 6,6,6,6                     | 0     |
| 56  | MG   | YA    | 3338 | 1/1   | 0.95 | 0.47 | 22.83 | 15,15,15,15                 | 0     |
| 56  | MG   | YA    | 3092 | 1/1   | 0.93 | 0.90 | 22.21 | 52,52,52,52                 | 0     |
| 56  | MG   | XA    | 1650 | 1/1   | 0.98 | 0.44 | 22.17 | 16,16,16,16                 | 0     |
| 56  | MG   | QA    | 1681 | 1/1   | 0.86 | 0.42 | 21.54 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3031 | 1/1   | 0.82 | 0.45 | 20.84 | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3405 | 1/1   | 0.82 | 0.31 | 20.79 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3026 | 1/1   | 0.97 | 0.54 | 20.33 | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3103 | 1/1   | 0.97 | 0.36 | 20.02 | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3425 | 1/1   | 0.71 | 0.84 | 19.53 | 62,62,62,62                 | 0     |
| 56  | MG   | YA    | 3122 | 1/1   | 0.96 | 0.49 | 19.32 | 14,14,14,14                 | 0     |
| 56  | MG   | RA    | 3128 | 1/1   | 0.84 | 0.41 | 19.31 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3255 | 1/1   | 0.93 | 0.61 | 19.20 | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3078 | 1/1   | 0.99 | 0.43 | 19.14 | 9,9,9,9                     | 0     |
| 56  | MG   | RA    | 3022 | 1/1   | 0.94 | 0.36 | 18.75 | 17,17,17,17                 | 0     |
| 56  | MG   | RA    | 3149 | 1/1   | 0.98 | 0.62 | 18.74 | 2,2,2,2                     | 0     |
| 56  | MG   | RA    | 3073 | 1/1   | 0.93 | 0.63 | 18.62 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | RA    | 3377 | 1/1   | 0.93 | 0.50 | 18.49 | 24,24,24,24                 | 0     |
| 56  | MG   | RA    | 3048 | 1/1   | 0.99 | 0.49 | 18.29 | 5,5,5,5                     | 0     |
| 56  | MG   | YA    | 3201 | 1/1   | 0.98 | 0.42 | 18.24 | 20,20,20,20                 | 0     |
| 56  | MG   | RA    | 3316 | 1/1   | 0.78 | 0.60 | 17.84 | 57,57,57,57                 | 0     |
| 56  | MG   | RA    | 3370 | 1/1   | 0.92 | 0.52 | 17.47 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3003 | 1/1   | 0.97 | 0.44 | 17.46 | 4,4,4,4                     | 0     |
| 56  | MG   | YA    | 3224 | 1/1   | 0.94 | 0.47 | 16.77 | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3017 | 1/1   | 0.96 | 0.70 | 16.73 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3209 | 1/1   | 0.91 | 0.47 | 16.56 | 19,19,19,19                 | 0     |
| 56  | MG   | RA    | 3425 | 1/1   | 0.90 | 0.40 | 16.51 | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3135 | 1/1   | 0.91 | 0.31 | 16.47 | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3336 | 1/1   | 0.98 | 0.45 | 16.46 | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3250 | 1/1   | 0.96 | 0.45 | 16.44 | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3240 | 1/1   | 0.89 | 0.35 | 16.39 | 17,17,17,17                 | 0     |
| 56  | MG   | RA    | 3050 | 1/1   | 0.94 | 0.37 | 16.32 | 6,6,6,6                     | 0     |
| 56  | MG   | YA    | 3414 | 1/1   | 0.95 | 0.68 | 16.22 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3006 | 1/1   | 0.98 | 0.49 | 16.00 | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3233 | 1/1   | 0.72 | 0.41 | 15.93 | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3037 | 1/1   | 0.74 | 0.67 | 15.91 | 24,24,24,24                 | 0     |
| 56  | MG   | RA    | 3295 | 1/1   | 0.75 | 0.41 | 15.91 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3291 | 1/1   | 0.98 | 0.33 | 15.68 | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3104 | 1/1   | 0.96 | 0.46 | 15.60 | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3167 | 1/1   | 0.94 | 0.32 | 15.53 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3094 | 1/1   | 0.96 | 0.66 | 15.16 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3233 | 1/1   | 0.87 | 0.40 | 15.12 | 25,25,25,25                 | 0     |
| 56  | MG   | QA    | 1741 | 1/1   | 0.92 | 0.44 | 14.84 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3467 | 1/1   | 0.70 | 0.45 | 14.66 | 68,68,68,68                 | 0     |
| 56  | MG   | QA    | 1606 | 1/1   | 0.90 | 0.30 | 14.42 | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3213 | 1/1   | 0.89 | 0.42 | 14.19 | 21,21,21,21                 | 0     |
| 56  | MG   | YA    | 3101 | 1/1   | 0.93 | 0.38 | 14.19 | 25,25,25,25                 | 0     |
| 56  | MG   | RA    | 3103 | 1/1   | 0.93 | 0.43 | 14.10 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3170 | 1/1   | 0.97 | 0.41 | 14.09 | 7,7,7,7                     | 0     |
| 56  | MG   | YA    | 3428 | 1/1   | 0.93 | 0.56 | 14.08 | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3193 | 1/1   | 0.98 | 0.33 | 14.03 | 0,0,0,0                     | 0     |
| 56  | MG   | RA    | 3099 | 1/1   | 0.91 | 0.49 | 14.03 | 25,25,25,25                 | 0     |
| 56  | MG   | RA    | 3095 | 1/1   | 0.91 | 0.52 | 13.88 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3459 | 1/1   | 0.71 | 0.51 | 13.84 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3028 | 1/1   | 0.97 | 0.49 | 13.35 | 10,10,10,10                 | 0     |
| 56  | MG   | QA    | 1656 | 1/1   | 0.99 | 0.46 | 13.10 | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3392 | 1/1   | 0.81 | 0.56 | 13.00 | 60,60,60,60                 | 0     |
| 56  | MG   | RA    | 3110 | 1/1   | 0.97 | 0.44 | 12.90 | 8,8,8,8                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | YA    | 3186 | 1/1   | 0.97 | 0.39 | 12.71 | 1,1,1,1                     | 0     |
| 56  | MG   | YA    | 3426 | 1/1   | 0.84 | 0.35 | 12.64 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3228 | 1/1   | 0.98 | 0.42 | 12.40 | 18,18,18,18                 | 0     |
| 56  | MG   | YA    | 3072 | 1/1   | 0.97 | 0.36 | 12.33 | 19,19,19,19                 | 0     |
| 56  | MG   | RA    | 3376 | 1/1   | 0.96 | 0.32 | 12.09 | 5,5,5,5                     | 0     |
| 56  | MG   | RA    | 3430 | 1/1   | 0.82 | 0.70 | 12.05 | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3318 | 1/1   | 0.84 | 0.32 | 11.98 | 32,32,32,32                 | 0     |
| 56  | MG   | XA    | 1643 | 1/1   | 0.95 | 0.35 | 11.97 | 23,23,23,23                 | 0     |
| 56  | MG   | QA    | 1637 | 1/1   | 0.91 | 0.47 | 11.77 | 53,53,53,53                 | 0     |
| 56  | MG   | QA    | 1608 | 1/1   | 0.92 | 0.55 | 11.77 | 25,25,25,25                 | 0     |
| 56  | MG   | QA    | 1682 | 1/1   | 0.83 | 0.61 | 11.75 | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3007 | 1/1   | 0.99 | 0.30 | 11.42 | 5,5,5,5                     | 0     |
| 56  | MG   | YF    | 301  | 1/1   | 0.88 | 0.65 | 11.13 | 37,37,37,37                 | 0     |
| 56  | MG   | QA    | 1719 | 1/1   | 0.74 | 0.47 | 10.98 | 70,70,70,70                 | 0     |
| 56  | MG   | RA    | 3065 | 1/1   | 0.97 | 0.41 | 10.94 | 10,10,10,10                 | 0     |
| 56  | MG   | XA    | 1742 | 1/1   | 0.95 | 0.43 | 10.87 | 73,73,73,73                 | 0     |
| 56  | MG   | RA    | 3125 | 1/1   | 0.92 | 0.31 | 10.86 | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3111 | 1/1   | 0.93 | 0.25 | 10.84 | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3127 | 1/1   | 0.88 | 0.33 | 10.78 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3340 | 1/1   | 0.94 | 0.53 | 10.78 | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3177 | 1/1   | 0.99 | 0.31 | 10.77 | 16,16,16,16                 | 0     |
| 56  | MG   | RA    | 3067 | 1/1   | 0.98 | 0.41 | 10.73 | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3057 | 1/1   | 0.97 | 0.52 | 10.62 | 2,2,2,2                     | 0     |
| 56  | MG   | YA    | 3038 | 1/1   | 0.91 | 0.59 | 10.58 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3056 | 1/1   | 0.98 | 0.47 | 10.56 | 1,1,1,1                     | 0     |
| 56  | MG   | RA    | 3247 | 1/1   | 0.92 | 0.34 | 10.49 | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3066 | 1/1   | 0.99 | 0.35 | 10.47 | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3044 | 1/1   | 0.98 | 0.33 | 10.30 | 12,12,12,12                 | 0     |
| 56  | MG   | RA    | 3264 | 1/1   | 0.86 | 0.33 | 10.13 | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3032 | 1/1   | 0.99 | 0.28 | 10.09 | 5,5,5,5                     | 0     |
| 56  | MG   | RQ    | 202  | 1/1   | 0.75 | 0.52 | 10.08 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3083 | 1/1   | 0.76 | 0.26 | 10.05 | 5,5,5,5                     | 0     |
| 56  | MG   | RA    | 3051 | 1/1   | 0.73 | 0.37 | 10.02 | 62,62,62,62                 | 0     |
| 56  | MG   | XA    | 1664 | 1/1   | 0.98 | 0.40 | 10.00 | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3416 | 1/1   | 0.48 | 0.27 | 9.92  | 9,9,9,9                     | 0     |
| 56  | MG   | YA    | 3027 | 1/1   | 0.97 | 0.42 | 9.90  | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3282 | 1/1   | 0.93 | 0.55 | 9.86  | 49,49,49,49                 | 0     |
| 56  | MG   | XA    | 1667 | 1/1   | 0.92 | 0.32 | 9.82  | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3027 | 1/1   | 0.97 | 0.42 | 9.74  | 2,2,2,2                     | 0     |
| 56  | MG   | RA    | 3018 | 1/1   | 0.95 | 0.44 | 9.68  | 10,10,10,10                 | 0     |
| 56  | MG   | YA    | 3203 | 1/1   | 0.96 | 0.25 | 9.66  | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | QA    | 1670 | 1/1   | 0.92 | 0.37 | 9.58 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3001 | 1/1   | 0.96 | 0.34 | 9.45 | 41,41,41,41                 | 0     |
| 56  | MG   | XA    | 1605 | 1/1   | 0.98 | 0.26 | 9.43 | 6,6,6,6                     | 0     |
| 56  | MG   | RA    | 3045 | 1/1   | 0.98 | 0.37 | 9.22 | 4,4,4,4                     | 0     |
| 56  | MG   | YA    | 3064 | 1/1   | 0.99 | 0.33 | 9.15 | 5,5,5,5                     | 0     |
| 56  | MG   | XA    | 1635 | 1/1   | 0.97 | 0.53 | 9.14 | 36,36,36,36                 | 0     |
| 56  | MG   | QA    | 1639 | 1/1   | 0.93 | 0.30 | 9.06 | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3432 | 1/1   | 0.89 | 0.29 | 9.01 | 91,91,91,91                 | 0     |
| 56  | MG   | RA    | 3222 | 1/1   | 0.75 | 0.43 | 8.99 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3070 | 1/1   | 0.96 | 0.34 | 8.97 | 3,3,3,3                     | 0     |
| 56  | MG   | RA    | 3108 | 1/1   | 0.78 | 0.61 | 8.90 | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3033 | 1/1   | 0.98 | 0.35 | 8.84 | 8,8,8,8                     | 0     |
| 56  | MG   | YA    | 3227 | 1/1   | 0.72 | 0.37 | 8.77 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3116 | 1/1   | 0.89 | 0.32 | 8.74 | 18,18,18,18                 | 0     |
| 56  | MG   | QA    | 1619 | 1/1   | 0.98 | 0.41 | 8.54 | 12,12,12,12                 | 0     |
| 56  | MG   | XA    | 1611 | 1/1   | 0.85 | 0.46 | 8.46 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3305 | 1/1   | 0.94 | 0.30 | 8.42 | 21,21,21,21                 | 0     |
| 56  | MG   | YA    | 3208 | 1/1   | 0.95 | 0.50 | 8.37 | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3013 | 1/1   | 0.86 | 0.26 | 8.31 | 0,0,0,0                     | 0     |
| 56  | MG   | YA    | 3147 | 1/1   | 0.95 | 0.59 | 8.29 | 1,1,1,1                     | 0     |
| 56  | MG   | XA    | 1625 | 1/1   | 0.25 | 0.29 | 8.29 | 80,80,80,80                 | 0     |
| 56  | MG   | QA    | 1643 | 1/1   | 0.90 | 0.27 | 8.10 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3074 | 1/1   | 0.97 | 0.44 | 8.00 | 27,27,27,27                 | 0     |
| 56  | MG   | XA    | 1613 | 1/1   | 0.91 | 0.24 | 7.91 | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3385 | 1/1   | 0.98 | 0.35 | 7.89 | 2,2,2,2                     | 0     |
| 56  | MG   | RA    | 3004 | 1/1   | 0.96 | 0.43 | 7.85 | 16,16,16,16                 | 0     |
| 56  | MG   | RA    | 3431 | 1/1   | 0.89 | 0.29 | 7.84 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3010 | 1/1   | 0.98 | 0.25 | 7.83 | 4,4,4,4                     | 0     |
| 56  | MG   | QA    | 1728 | 1/1   | 0.70 | 0.25 | 7.82 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3055 | 1/1   | 0.96 | 0.25 | 7.82 | 12,12,12,12                 | 0     |
| 56  | MG   | YA    | 3082 | 1/1   | 0.82 | 0.27 | 7.80 | 20,20,20,20                 | 0     |
| 56  | MG   | QA    | 1641 | 1/1   | 0.96 | 0.46 | 7.77 | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3011 | 1/1   | 0.97 | 0.51 | 7.76 | 0,0,0,0                     | 0     |
| 56  | MG   | XA    | 1754 | 1/1   | 0.90 | 0.36 | 7.74 | 55,55,55,55                 | 0     |
| 56  | MG   | XA    | 1624 | 1/1   | 0.91 | 0.37 | 7.72 | 59,59,59,59                 | 0     |
| 56  | MG   | YA    | 3146 | 1/1   | 0.95 | 0.38 | 7.66 | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3102 | 1/1   | 0.92 | 0.40 | 7.64 | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3249 | 1/1   | 0.85 | 0.41 | 7.62 | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3234 | 1/1   | 0.91 | 0.25 | 7.58 | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3209 | 1/1   | 0.99 | 0.30 | 7.56 | 9,9,9,9                     | 0     |
| 56  | MG   | RA    | 3368 | 1/1   | 0.84 | 0.36 | 7.46 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3407 | 1/1   | 0.96 | 0.34 | 7.43 | 4,4,4,4                     | 0     |
| 56  | MG   | RA    | 3140 | 1/1   | 0.97 | 0.31 | 7.23 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3034 | 1/1   | 0.99 | 0.35 | 7.17 | 9,9,9,9                     | 0     |
| 56  | MG   | YA    | 3109 | 1/1   | 0.97 | 0.44 | 7.16 | 14,14,14,14                 | 0     |
| 56  | MG   | RA    | 3365 | 1/1   | 0.87 | 0.34 | 7.11 | 21,21,21,21                 | 0     |
| 56  | MG   | QA    | 1609 | 1/1   | 0.95 | 0.31 | 7.04 | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3026 | 1/1   | 0.92 | 0.39 | 6.85 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3357 | 1/1   | 0.75 | 0.28 | 6.83 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3099 | 1/1   | 0.59 | 0.52 | 6.80 | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3013 | 1/1   | 0.99 | 0.31 | 6.30 | 0,0,0,0                     | 0     |
| 56  | MG   | YA    | 3191 | 1/1   | 0.97 | 0.40 | 6.29 | 9,9,9,9                     | 0     |
| 56  | MG   | RA    | 3386 | 1/1   | 0.94 | 0.23 | 6.26 | 17,17,17,17                 | 0     |
| 56  | MG   | RA    | 3148 | 1/1   | 0.83 | 0.23 | 6.16 | 19,19,19,19                 | 0     |
| 56  | MG   | RA    | 3159 | 1/1   | 0.99 | 0.36 | 6.12 | 5,5,5,5                     | 0     |
| 56  | MG   | XA    | 1618 | 1/1   | 0.94 | 0.31 | 6.09 | 15,15,15,15                 | 0     |
| 56  | MG   | RA    | 3296 | 1/1   | 0.91 | 0.20 | 6.09 | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3039 | 1/1   | 0.99 | 0.29 | 6.02 | 21,21,21,21                 | 0     |
| 56  | MG   | QA    | 1632 | 1/1   | 0.96 | 0.45 | 5.99 | 57,57,57,57                 | 0     |
| 56  | MG   | RA    | 3184 | 1/1   | 0.85 | 0.22 | 5.87 | 24,24,24,24                 | 0     |
| 56  | MG   | RA    | 3061 | 1/1   | 0.98 | 0.24 | 5.79 | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3033 | 1/1   | 0.98 | 0.26 | 5.68 | 10,10,10,10                 | 0     |
| 56  | MG   | YA    | 3097 | 1/1   | 0.93 | 0.32 | 5.67 | 21,21,21,21                 | 0     |
| 56  | MG   | RA    | 3198 | 1/1   | 0.96 | 0.28 | 5.65 | 26,26,26,26                 | 0     |
| 56  | MG   | QA    | 1636 | 1/1   | 0.74 | 0.43 | 5.58 | 56,56,56,56                 | 0     |
| 56  | MG   | XA    | 1604 | 1/1   | 0.97 | 0.28 | 5.51 | 9,9,9,9                     | 0     |
| 56  | MG   | XA    | 1607 | 1/1   | 0.89 | 0.52 | 5.49 | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3105 | 1/1   | 0.90 | 0.32 | 5.47 | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3014 | 1/1   | 0.90 | 0.27 | 5.41 | 3,3,3,3                     | 0     |
| 56  | MG   | YA    | 3204 | 1/1   | 0.95 | 0.20 | 5.38 | 10,10,10,10                 | 0     |
| 56  | MG   | YA    | 3071 | 1/1   | 0.95 | 0.20 | 5.34 | 17,17,17,17                 | 0     |
| 56  | MG   | RA    | 3427 | 1/1   | 0.86 | 0.40 | 5.31 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3071 | 1/1   | 0.97 | 0.28 | 5.31 | 9,9,9,9                     | 0     |
| 56  | MG   | XA    | 1692 | 1/1   | 0.96 | 0.25 | 5.30 | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3012 | 1/1   | 0.96 | 0.28 | 5.24 | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3062 | 1/1   | 0.99 | 0.26 | 5.14 | 0,0,0,0                     | 0     |
| 56  | MG   | YA    | 3210 | 1/1   | 0.91 | 0.28 | 4.99 | 25,25,25,25                 | 0     |
| 56  | MG   | RD    | 302  | 1/1   | 0.98 | 0.35 | 4.97 | 9,9,9,9                     | 0     |
| 56  | MG   | QA    | 1605 | 1/1   | 0.98 | 0.28 | 4.95 | 31,31,31,31                 | 0     |
| 56  | MG   | R5    | 102  | 1/1   | 0.93 | 0.38 | 4.95 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3343 | 1/1   | 0.72 | 0.40 | 4.91 | 61,61,61,61                 | 0     |
| 56  | MG   | YA    | 3221 | 1/1   | 0.93 | 0.22 | 4.78 | 16,16,16,16                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3107 | 1/1   | 0.95 | 0.26 | 4.73 | 20,20,20,20                 | 0     |
| 56  | MG   | RA    | 3306 | 1/1   | 0.92 | 0.67 | 4.72 | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3424 | 1/1   | 0.91 | 0.24 | 4.67 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3276 | 1/1   | 0.89 | 0.34 | 4.57 | 31,31,31,31                 | 0     |
| 56  | MG   | XA    | 1640 | 1/1   | 0.99 | 0.34 | 4.49 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3042 | 1/1   | 0.96 | 0.38 | 4.31 | 7,7,7,7                     | 0     |
| 56  | MG   | RA    | 3072 | 1/1   | 0.94 | 0.34 | 4.25 | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3407 | 1/1   | 0.98 | 0.31 | 4.23 | 4,4,4,4                     | 0     |
| 56  | MG   | RA    | 3350 | 1/1   | 0.96 | 0.24 | 4.22 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3018 | 1/1   | 0.98 | 0.22 | 4.14 | 18,18,18,18                 | 0     |
| 56  | MG   | QA    | 1651 | 1/1   | 0.97 | 0.19 | 4.01 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3339 | 1/1   | 0.87 | 0.25 | 3.96 | 62,62,62,62                 | 0     |
| 56  | MG   | RA    | 3155 | 1/1   | 0.98 | 0.24 | 3.96 | 12,12,12,12                 | 0     |
| 56  | MG   | YA    | 3066 | 1/1   | 0.97 | 0.29 | 3.94 | 27,27,27,27                 | 0     |
| 56  | MG   | QA    | 1699 | 1/1   | 0.77 | 0.28 | 3.94 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3073 | 1/1   | 0.97 | 0.34 | 3.93 | 15,15,15,15                 | 0     |
| 56  | MG   | RA    | 3153 | 1/1   | 0.89 | 0.23 | 3.92 | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3485 | 1/1   | 0.74 | 0.29 | 3.91 | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3151 | 1/1   | 0.91 | 0.22 | 3.90 | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3137 | 1/1   | 0.92 | 0.22 | 3.88 | 5,5,5,5                     | 0     |
| 56  | MG   | QA    | 1601 | 1/1   | 0.98 | 0.25 | 3.82 | 17,17,17,17                 | 0     |
| 56  | MG   | QA    | 1729 | 1/1   | 0.84 | 0.27 | 3.76 | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3473 | 1/1   | 0.88 | 0.20 | 3.70 | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3106 | 1/1   | 0.93 | 0.27 | 3.70 | 15,15,15,15                 | 0     |
| 56  | MG   | RA    | 3225 | 1/1   | 0.90 | 0.33 | 3.60 | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1625 | 1/1   | 0.97 | 0.32 | 3.55 | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3434 | 1/1   | 0.92 | 0.21 | 3.54 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3130 | 1/1   | 0.91 | 0.21 | 3.51 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3431 | 1/1   | 0.95 | 0.18 | 3.49 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3121 | 1/1   | 0.81 | 0.23 | 3.42 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3060 | 1/1   | 0.98 | 0.27 | 3.41 | 3,3,3,3                     | 0     |
| 56  | MG   | RA    | 3206 | 1/1   | 0.82 | 0.24 | 3.41 | 18,18,18,18                 | 0     |
| 56  | MG   | YA    | 3079 | 1/1   | 0.96 | 0.24 | 3.40 | 34,34,34,34                 | 0     |
| 56  | MG   | QA    | 1604 | 1/1   | 0.98 | 0.27 | 3.40 | 17,17,17,17                 | 0     |
| 56  | MG   | RA    | 3339 | 1/1   | 0.91 | 0.26 | 3.39 | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3205 | 1/1   | 0.95 | 0.23 | 3.38 | 19,19,19,19                 | 0     |
| 56  | MG   | RA    | 3080 | 1/1   | 1.00 | 0.27 | 3.31 | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3155 | 1/1   | 0.78 | 0.24 | 3.30 | 41,41,41,41                 | 0     |
| 56  | MG   | Y1    | 101  | 1/1   | 0.95 | 0.37 | 3.22 | 24,24,24,24                 | 0     |
| 56  | MG   | QA    | 1644 | 1/1   | 0.97 | 0.24 | 3.18 | 23,23,23,23                 | 0     |
| 56  | MG   | XA    | 1638 | 1/1   | 0.95 | 0.33 | 3.13 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | XA    | 1745 | 1/1   | 0.86 | 0.23 | 3.07 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3463 | 1/1   | 0.75 | 0.37 | 3.01 | 53,53,53,53                 | 0     |
| 56  | MG   | QA    | 1687 | 1/1   | 0.95 | 0.25 | 2.95 | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3220 | 1/1   | 0.88 | 0.16 | 2.93 | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3088 | 1/1   | 0.95 | 0.21 | 2.93 | 5,5,5,5                     | 0     |
| 56  | MG   | YQ    | 201  | 1/1   | 0.84 | 0.31 | 2.91 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3484 | 1/1   | 0.80 | 0.30 | 2.86 | 24,24,24,24                 | 0     |
| 56  | MG   | RA    | 3056 | 1/1   | 0.98 | 0.20 | 2.83 | 14,14,14,14                 | 0     |
| 56  | MG   | RA    | 3436 | 1/1   | 0.95 | 0.30 | 2.80 | 8,8,8,8                     | 0     |
| 56  | MG   | XA    | 1695 | 1/1   | 0.94 | 0.24 | 2.79 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3202 | 1/1   | 0.93 | 0.21 | 2.79 | 22,22,22,22                 | 0     |
| 56  | MG   | XA    | 1755 | 1/1   | 0.54 | 0.30 | 2.72 | 68,68,68,68                 | 0     |
| 56  | MG   | YA    | 3418 | 1/1   | 0.94 | 0.17 | 2.71 | 16,16,16,16                 | 0     |
| 56  | MG   | XA    | 1697 | 1/1   | 0.92 | 0.25 | 2.71 | 42,42,42,42                 | 0     |
| 56  | MG   | XA    | 1659 | 1/1   | 0.97 | 0.42 | 2.68 | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3254 | 1/1   | 0.94 | 0.20 | 2.66 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3133 | 1/1   | 0.90 | 0.18 | 2.60 | 25,25,25,25                 | 0     |
| 56  | MG   | RA    | 3420 | 1/1   | 0.94 | 0.22 | 2.59 | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3011 | 1/1   | 0.99 | 0.19 | 2.59 | 1,1,1,1                     | 0     |
| 56  | MG   | QA    | 1703 | 1/1   | 0.80 | 0.21 | 2.58 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3438 | 1/1   | 0.89 | 0.23 | 2.54 | 23,23,23,23                 | 0     |
| 56  | MG   | RA    | 3047 | 1/1   | 0.98 | 0.23 | 2.54 | 25,25,25,25                 | 0     |
| 56  | MG   | RA    | 3166 | 1/1   | 0.76 | 0.23 | 2.51 | 31,31,31,31                 | 0     |
| 56  | MG   | XA    | 1717 | 1/1   | 0.84 | 0.45 | 2.50 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3156 | 1/1   | 0.96 | 0.36 | 2.49 | 15,15,15,15                 | 0     |
| 56  | MG   | RA    | 3131 | 1/1   | 0.88 | 0.24 | 2.42 | 78,78,78,78                 | 0     |
| 56  | MG   | RA    | 3197 | 1/1   | 0.90 | 0.21 | 2.42 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3355 | 1/1   | 0.47 | 0.30 | 2.41 | 58,58,58,58                 | 0     |
| 56  | MG   | QA    | 1645 | 1/1   | 0.96 | 0.25 | 2.40 | 41,41,41,41                 | 0     |
| 56  | MG   | XA    | 1601 | 1/1   | 0.99 | 0.22 | 2.39 | 8,8,8,8                     | 0     |
| 56  | MG   | XA    | 1644 | 1/1   | 0.94 | 0.22 | 2.38 | 25,25,25,25                 | 0     |
| 56  | MG   | QA    | 1662 | 1/1   | 0.83 | 0.23 | 2.35 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3264 | 1/1   | 0.97 | 0.29 | 2.28 | 16,16,16,16                 | 0     |
| 56  | MG   | QA    | 1668 | 1/1   | 0.91 | 0.21 | 2.26 | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3251 | 1/1   | 0.88 | 0.24 | 2.16 | 63,63,63,63                 | 0     |
| 56  | MG   | YD    | 301  | 1/1   | 0.98 | 0.44 | 2.15 | 2,2,2,2                     | 0     |
| 56  | MG   | RA    | 3259 | 1/1   | 0.79 | 0.24 | 2.11 | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3053 | 1/1   | 0.95 | 0.18 | 2.08 | 21,21,21,21                 | 0     |
| 56  | MG   | QA    | 1614 | 1/1   | 0.92 | 0.19 | 1.92 | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1741 | 1/1   | 0.87 | 0.23 | 1.83 | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3093 | 1/1   | 0.98 | 0.23 | 1.70 | 17,17,17,17                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3111 | 1/1   | 0.84 | 0.21 | 1.60 | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3050 | 1/1   | 0.93 | 0.19 | 1.59 | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3136 | 1/1   | 0.92 | 0.21 | 1.58 | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3172 | 1/1   | 0.89 | 0.18 | 1.57 | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3240 | 1/1   | 0.92 | 0.20 | 1.55 | 26,26,26,26                 | 0     |
| 56  | MG   | XA    | 1748 | 1/1   | 0.94 | 0.23 | 1.54 | 66,66,66,66                 | 0     |
| 56  | MG   | YA    | 3090 | 1/1   | 0.86 | 0.21 | 1.49 | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3298 | 1/1   | 0.94 | 0.21 | 1.48 | 21,21,21,21                 | 0     |
| 56  | MG   | YA    | 3005 | 1/1   | 0.96 | 0.23 | 1.45 | 1,1,1,1                     | 0     |
| 56  | MG   | YA    | 3327 | 1/1   | 0.97 | 0.17 | 1.36 | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3164 | 1/1   | 0.93 | 0.23 | 1.32 | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3347 | 1/1   | 0.89 | 0.27 | 1.30 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3046 | 1/1   | 0.90 | 0.24 | 1.27 | 14,14,14,14                 | 0     |
| 56  | MG   | XA    | 1736 | 1/1   | 0.93 | 0.20 | 1.25 | 23,23,23,23                 | 0     |
| 56  | MG   | QA    | 1738 | 1/1   | 0.92 | 0.16 | 1.24 | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3444 | 1/1   | 0.96 | 0.27 | 1.17 | 5,5,5,5                     | 0     |
| 56  | MG   | RA    | 3030 | 1/1   | 0.95 | 0.20 | 1.13 | 13,13,13,13                 | 0     |
| 56  | MG   | YA    | 3286 | 1/1   | 0.97 | 0.18 | 0.99 | 20,20,20,20                 | 0     |
| 56  | MG   | YA    | 3032 | 1/1   | 0.97 | 0.23 | 0.94 | 16,16,16,16                 | 0     |
| 56  | MG   | QA    | 1626 | 1/1   | 0.80 | 0.17 | 0.91 | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3228 | 1/1   | 0.97 | 0.17 | 0.89 | 25,25,25,25                 | 0     |
| 56  | MG   | QA    | 1693 | 1/1   | 0.76 | 0.17 | 0.88 | 66,66,66,66                 | 0     |
| 56  | MG   | XA    | 1603 | 1/1   | 0.98 | 0.20 | 0.88 | 24,24,24,24                 | 0     |
| 57  | ZN   | XD    | 301  | 1/1   | 0.88 | 0.37 | 0.85 | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3356 | 1/1   | 0.97 | 0.19 | 0.84 | 30,30,30,30                 | 0     |
| 56  | MG   | RR    | 201  | 1/1   | 0.89 | 0.28 | 0.78 | 31,31,31,31                 | 0     |
| 57  | ZN   | QD    | 301  | 1/1   | 0.97 | 0.33 | 0.74 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3471 | 1/1   | 0.87 | 0.21 | 0.62 | 28,28,28,28                 | 0     |
| 56  | MG   | XA    | 1743 | 1/1   | 0.90 | 0.16 | 0.61 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3059 | 1/1   | 0.99 | 0.20 | 0.56 | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3434 | 1/1   | 0.94 | 0.19 | 0.52 | 42,42,42,42                 | 0     |
| 56  | MG   | XA    | 1614 | 1/1   | 0.96 | 0.22 | 0.46 | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3456 | 1/1   | 0.81 | 0.21 | 0.43 | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3237 | 1/1   | 0.93 | 0.18 | 0.41 | 23,23,23,23                 | 0     |
| 56  | MG   | XS    | 300  | 1/1   | 0.95 | 0.31 | 0.38 | 29,29,29,29                 | 0     |
| 56  | MG   | QA    | 1673 | 1/1   | 0.88 | 0.33 | 0.37 | 70,70,70,70                 | 0     |
| 56  | MG   | XA    | 1656 | 1/1   | 0.70 | 0.17 | 0.36 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3131 | 1/1   | 0.96 | 0.17 | 0.35 | 11,11,11,11                 | 0     |
| 56  | MG   | YA    | 3164 | 1/1   | 0.85 | 0.16 | 0.35 | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1761 | 1/1   | 0.87 | 0.20 | 0.26 | 23,23,23,23                 | 0     |
| 56  | MG   | QA    | 1628 | 1/1   | 0.82 | 0.24 | 0.26 | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3060 | 1/1   | 0.83 | 0.15 | 0.20 | 14,14,14,14                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | RA    | 3235 | 1/1   | 0.92 | 0.20 | 0.18  | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3021 | 1/1   | 0.96 | 0.20 | 0.16  | 17,17,17,17                 | 0     |
| 56  | MG   | XA    | 1732 | 1/1   | 0.97 | 0.14 | 0.16  | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3161 | 1/1   | 0.92 | 0.19 | 0.15  | 39,39,39,39                 | 0     |
| 56  | MG   | XV    | 101  | 1/1   | 0.97 | 0.20 | 0.14  | 39,39,39,39                 | 0     |
| 56  | MG   | XA    | 1634 | 1/1   | 0.92 | 0.20 | 0.12  | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3298 | 1/1   | 0.80 | 0.17 | 0.11  | 52,52,52,52                 | 0     |
| 56  | MG   | QA    | 1725 | 1/1   | 0.85 | 0.18 | 0.08  | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3439 | 1/1   | 0.82 | 0.26 | 0.08  | 50,50,50,50                 | 0     |
| 56  | MG   | QA    | 1654 | 1/1   | 0.98 | 0.22 | 0.05  | 20,20,20,20                 | 0     |
| 56  | MG   | RD    | 301  | 1/1   | 0.92 | 0.21 | 0.03  | 24,24,24,24                 | 0     |
| 56  | MG   | RA    | 3424 | 1/1   | 0.96 | 0.16 | -0.03 | 26,26,26,26                 | 0     |
| 56  | MG   | RP    | 201  | 1/1   | 0.96 | 0.25 | -0.03 | 21,21,21,21                 | 0     |
| 56  | MG   | QA    | 1750 | 1/1   | 0.71 | 0.23 | -0.04 | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3157 | 1/1   | 0.76 | 0.19 | -0.04 | 43,43,43,43                 | 0     |
| 56  | MG   | XA    | 1642 | 1/1   | 0.98 | 0.18 | -0.05 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3283 | 1/1   | 0.94 | 0.18 | -0.07 | 18,18,18,18                 | 0     |
| 56  | MG   | YA    | 3008 | 1/1   | 0.99 | 0.17 | -0.12 | 2,2,2,2                     | 0     |
| 56  | MG   | RA    | 3162 | 1/1   | 0.85 | 0.20 | -0.15 | 49,49,49,49                 | 0     |
| 56  | MG   | QA    | 1744 | 1/1   | 0.93 | 0.16 | -0.20 | 56,56,56,56                 | 0     |
| 56  | MG   | RA    | 3351 | 1/1   | 0.83 | 0.21 | -0.20 | 75,75,75,75                 | 0     |
| 56  | MG   | RA    | 3281 | 1/1   | 0.84 | 0.16 | -0.25 | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3128 | 1/1   | 0.86 | 0.17 | -0.27 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3244 | 1/1   | 0.86 | 0.17 | -0.31 | 54,54,54,54                 | 0     |
| 56  | MG   | QD    | 303  | 1/1   | 0.13 | 0.16 | -0.40 | 69,69,69,69                 | 0     |
| 56  | MG   | QV    | 104  | 1/1   | 0.96 | 0.17 | -0.44 | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3437 | 1/1   | 0.95 | 0.18 | -0.46 | 24,24,24,24                 | 0     |
| 56  | MG   | XA    | 1653 | 1/1   | 0.97 | 0.14 | -0.48 | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3284 | 1/1   | 0.98 | 0.17 | -0.49 | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3104 | 1/1   | 0.98 | 0.16 | -0.49 | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3009 | 1/1   | 0.97 | 0.15 | -0.50 | 6,6,6,6                     | 0     |
| 56  | MG   | YA    | 3420 | 1/1   | 0.89 | 0.17 | -0.52 | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3108 | 1/1   | 0.92 | 0.17 | -0.55 | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3132 | 1/1   | 0.90 | 0.17 | -0.62 | 20,20,20,20                 | 0     |
| 56  | MG   | QA    | 1742 | 1/1   | 0.88 | 0.15 | -0.62 | 22,22,22,22                 | 0     |
| 56  | MG   | QA    | 1666 | 1/1   | 0.94 | 0.13 | -0.63 | 23,23,23,23                 | 0     |
| 56  | MG   | QA    | 1678 | 1/1   | 0.92 | 0.15 | -0.65 | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3337 | 1/1   | 0.97 | 0.14 | -0.68 | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3218 | 1/1   | 0.92 | 0.13 | -0.73 | 36,36,36,36                 | 0     |
| 56  | MG   | XA    | 1679 | 1/1   | 0.97 | 0.13 | -0.75 | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3429 | 1/1   | 0.92 | 0.14 | -0.80 | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3294 | 1/1   | 0.82 | 0.13 | -0.82 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | XA    | 1627 | 1/1   | 0.83 | 0.17 | -0.85 | 57,57,57,57                 | 0     |
| 56  | MG   | RA    | 3279 | 1/1   | 0.87 | 0.17 | -0.90 | 26,26,26,26                 | 0     |
| 56  | MG   | XF    | 201  | 1/1   | 0.86 | 0.18 | -0.91 | 39,39,39,39                 | 0     |
| 56  | MG   | QA    | 1615 | 1/1   | 0.93 | 0.14 | -0.95 | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3206 | 1/1   | 0.95 | 0.15 | -0.97 | 12,12,12,12                 | 0     |
| 56  | MG   | YA    | 3474 | 1/1   | 0.96 | 0.13 | -1.01 | 23,23,23,23                 | 0     |
| 56  | MG   | XD    | 302  | 1/1   | 0.65 | 0.14 | -1.04 | 85,85,85,85                 | 0     |
| 56  | MG   | XA    | 1762 | 1/1   | 0.96 | 0.17 | -1.11 | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3085 | 1/1   | 0.99 | 0.12 | -1.12 | 13,13,13,13                 | 0     |
| 56  | MG   | YG    | 201  | 1/1   | 0.64 | 0.14 | -1.14 | 56,56,56,56                 | 0     |
| 56  | MG   | Y5    | 103  | 1/1   | 0.97 | 0.15 | -1.17 | 41,41,41,41                 | 0     |
| 56  | MG   | RP    | 202  | 1/1   | 0.92 | 0.17 | -1.24 | 18,18,18,18                 | 0     |
| 56  | MG   | YA    | 3200 | 1/1   | 0.97 | 0.11 | -1.24 | 1,1,1,1                     | 0     |
| 56  | MG   | QA    | 1730 | 1/1   | 0.97 | 0.15 | -1.28 | 58,58,58,58                 | 0     |
| 57  | ZN   | XN    | 101  | 1/1   | 0.93 | 0.13 | -1.31 | 67,67,67,67                 | 0     |
| 56  | MG   | QA    | 1749 | 1/1   | 0.93 | 0.13 | -1.32 | 41,41,41,41                 | 0     |
| 57  | ZN   | QN    | 101  | 1/1   | 0.95 | 0.14 | -1.33 | 76,76,76,76                 | 0     |
| 56  | MG   | XA    | 1620 | 1/1   | 0.79 | 0.15 | -1.34 | 21,21,21,21                 | 0     |
| 56  | MG   | XA    | 1763 | 1/1   | 0.83 | 0.15 | -1.34 | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3129 | 1/1   | 0.95 | 0.13 | -1.36 | 14,14,14,14                 | 0     |
| 56  | MG   | XA    | 1690 | 1/1   | 0.98 | 0.13 | -1.40 | 65,65,65,65                 | 0     |
| 56  | MG   | XA    | 1623 | 1/1   | 0.95 | 0.12 | -1.46 | 20,20,20,20                 | 0     |
| 56  | MG   | YA    | 3248 | 1/1   | 0.88 | 0.10 | -1.56 | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3440 | 1/1   | 0.86 | 0.11 | -1.57 | 12,12,12,12                 | 0     |
| 56  | MG   | XA    | 1734 | 1/1   | 0.90 | 0.10 | -1.72 | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3212 | 1/1   | 0.97 | 0.10 | -1.73 | 32,32,32,32                 | 0     |
| 56  | MG   | YP    | 201  | 1/1   | 0.97 | 0.13 | -1.84 | 7,7,7,7                     | 0     |
| 56  | MG   | YA    | 3486 | 1/1   | 0.94 | 0.10 | -1.84 | 19,19,19,19                 | 0     |
| 56  | MG   | YB    | 205  | 1/1   | 0.95 | 0.12 | -1.86 | 48,48,48,48                 | 0     |
| 56  | MG   | QV    | 101  | 1/1   | 0.91 | 0.12 | -1.86 | 31,31,31,31                 | 0     |
| 56  | MG   | R5    | 103  | 1/1   | 0.93 | 0.10 | -1.89 | 25,25,25,25                 | 0     |
| 56  | MG   | QA    | 1685 | 1/1   | 0.93 | 0.10 | -2.04 | 11,11,11,11                 | 0     |
| 56  | MG   | RP    | 203  | 1/1   | 0.95 | 0.17 | -2.08 | 4,4,4,4                     | 0     |
| 56  | MG   | RA    | 3174 | 1/1   | 0.91 | 0.10 | -2.10 | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3059 | 1/1   | 0.90 | 0.14 | -2.12 | 15,15,15,15                 | 0     |
| 56  | MG   | XA    | 1672 | 1/1   | 0.87 | 0.13 | -2.28 | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3421 | 1/1   | 0.80 | 0.09 | -2.36 | 68,68,68,68                 | 0     |
| 56  | MG   | YN    | 201  | 1/1   | 0.93 | 0.14 | -2.54 | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3121 | 1/1   | 0.88 | 0.12 | -2.56 | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3029 | 1/1   | 0.86 | 0.12 | -2.63 | 15,15,15,15                 | 0     |
| 56  | MG   | RB    | 204  | 1/1   | 0.82 | 0.09 | -2.78 | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3462 | 1/1   | 0.93 | 0.09 | -2.98 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56  | MG   | RA    | 3238 | 1/1   | 0.98 | 0.10 | -3.09 | 11,11,11,11                 | 0     |
| 56  | MG   | XA    | 1682 | 1/1   | 0.94 | 0.07 | -3.13 | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3243 | 1/1   | 0.97 | 0.12 | -3.25 | 37,37,37,37                 | 0     |
| 56  | MG   | QA    | 1726 | 1/1   | 0.97 | 0.10 | -3.45 | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3237 | 1/1   | 0.98 | 0.11 | -3.80 | 37,37,37,37                 | 0     |
| 56  | MG   | QA    | 1624 | 1/1   | 0.98 | 0.11 | -4.04 | 31,31,31,31                 | 0     |
| 56  | MG   | RF    | 301  | 1/1   | 0.93 | 0.10 | -4.11 | 24,24,24,24                 | 0     |
| 56  | MG   | RA    | 3141 | 1/1   | 0.81 | 0.09 | -4.14 | 31,31,31,31                 | 0     |
| 56  | MG   | QA    | 1688 | 1/1   | 0.94 | 0.10 | -4.19 | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3084 | 1/1   | 0.88 | 0.09 | -4.28 | 11,11,11,11                 | 0     |
| 56  | MG   | YA    | 3058 | 1/1   | 0.99 | 0.06 | -4.57 | 34,34,34,34                 | 0     |
| 56  | MG   | XA    | 1609 | 1/1   | 0.98 | 0.06 | -5.26 | 79,79,79,79                 | 0     |
| 56  | MG   | YA    | 3238 | 1/1   | 0.93 | 0.12 | -5.48 | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3138 | 1/1   | 0.96 | 0.05 | -5.56 | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3161 | 1/1   | 0.93 | 0.16 | -5.87 | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3006 | 1/1   | 0.97 | 0.07 | -6.36 | 0,0,0,0                     | 0     |
| 56  | MG   | YA    | 3171 | 1/1   | 0.94 | 0.09 | -6.81 | 26,26,26,26                 | 0     |
| 56  | MG   | YQ    | 202  | 1/1   | 0.93 | 0.29 | -     | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3016 | 1/1   | 0.96 | 0.07 | -     | 2,2,2,2                     | 0     |
| 56  | MG   | RA    | 3163 | 1/1   | 0.98 | 0.25 | -     | 34,34,34,34                 | 0     |
| 56  | MG   | XA    | 1723 | 1/1   | 0.91 | 0.38 | -     | 58,58,58,58                 | 0     |
| 56  | MG   | QA    | 1613 | 1/1   | 0.87 | 0.25 | -     | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3401 | 1/1   | 0.75 | 0.59 | -     | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3239 | 1/1   | 0.84 | 0.33 | -     | 40,40,40,40                 | 0     |
| 56  | MG   | XA    | 1731 | 1/1   | 0.82 | 0.15 | -     | 47,47,47,47                 | 0     |
| 56  | MG   | QL    | 201  | 1/1   | 0.89 | 0.26 | -     | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3397 | 1/1   | 0.92 | 0.57 | -     | 58,58,58,58                 | 0     |
| 56  | MG   | QA    | 1611 | 1/1   | 0.93 | 0.24 | -     | 28,28,28,28                 | 0     |
| 56  | MG   | QA    | 1717 | 1/1   | 0.94 | 0.77 | -     | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3016 | 1/1   | 0.98 | 0.30 | -     | 6,6,6,6                     | 0     |
| 56  | MG   | QV    | 103  | 1/1   | 0.86 | 0.26 | -     | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3133 | 1/1   | 0.96 | 0.33 | -     | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3442 | 1/1   | 0.97 | 0.28 | -     | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3413 | 1/1   | 0.95 | 0.26 | -     | 7,7,7,7                     | 0     |
| 56  | MG   | RA    | 3052 | 1/1   | 0.97 | 0.26 | -     | 4,4,4,4                     | 0     |
| 56  | MG   | RA    | 3367 | 1/1   | 0.94 | 0.16 | -     | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3203 | 1/1   | 0.96 | 0.25 | -     | 26,26,26,26                 | 0     |
| 56  | MG   | QA    | 1667 | 1/1   | 0.99 | 0.22 | -     | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3310 | 1/1   | 0.97 | 0.39 | -     | 17,17,17,17                 | 0     |
| 56  | MG   | QA    | 1712 | 1/1   | 0.90 | 0.32 | -     | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3341 | 1/1   | 0.95 | 0.16 | -     | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3398 | 1/1   | 0.82 | 0.29 | -     | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3070 | 1/1   | 0.92 | 0.32 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | R5    | 101  | 1/1   | 0.95 | 0.32 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3321 | 1/1   | 0.83 | 0.27 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3215 | 1/1   | 0.58 | 0.29 | -    | 79,79,79,79                 | 0     |
| 56  | MG   | RA    | 3204 | 1/1   | 0.68 | 0.36 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3482 | 1/1   | 0.73 | 0.42 | -    | 69,69,69,69                 | 0     |
| 56  | MG   | RA    | 3353 | 1/1   | 0.90 | 0.50 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | QA    | 1748 | 1/1   | 0.92 | 0.37 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3284 | 1/1   | 0.96 | 0.33 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3101 | 1/1   | 0.87 | 0.35 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | XA    | 1689 | 1/1   | 0.98 | 0.41 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3074 | 1/1   | 0.96 | 0.54 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | YA    | 3009 | 1/1   | 0.98 | 0.33 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | XA    | 1760 | 1/1   | 0.94 | 0.28 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3261 | 1/1   | 0.92 | 0.41 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3223 | 1/1   | 0.71 | 0.37 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3411 | 1/1   | 0.90 | 0.49 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3267 | 1/1   | 0.94 | 0.16 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3435 | 1/1   | 0.91 | 0.55 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3402 | 1/1   | 0.75 | 0.25 | -    | 70,70,70,70                 | 0     |
| 56  | MG   | RA    | 3087 | 1/1   | 0.99 | 0.23 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | RA    | 3260 | 1/1   | 0.97 | 0.37 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3176 | 1/1   | 0.93 | 0.18 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3273 | 1/1   | 0.96 | 0.18 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | XA    | 1706 | 1/1   | 0.85 | 0.26 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3378 | 1/1   | 0.98 | 0.37 | -    | 2,2,2,2                     | 0     |
| 56  | MG   | QA    | 1721 | 1/1   | 0.70 | 0.20 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3040 | 1/1   | 0.93 | 0.29 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | QA    | 1602 | 1/1   | 0.95 | 0.47 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | XA    | 1630 | 1/1   | 0.73 | 0.20 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1686 | 1/1   | 0.86 | 0.70 | -    | 72,72,72,72                 | 0     |
| 56  | MG   | YA    | 3364 | 1/1   | 0.92 | 0.80 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3450 | 1/1   | 0.95 | 0.23 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | QA    | 1627 | 1/1   | 0.61 | 0.80 | -    | 72,72,72,72                 | 0     |
| 56  | MG   | XA    | 1750 | 1/1   | 0.72 | 0.27 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3454 | 1/1   | 0.86 | 0.37 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | QA    | 1649 | 1/1   | 0.95 | 0.23 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3069 | 1/1   | 0.94 | 0.46 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | XA    | 1615 | 1/1   | 0.96 | 0.31 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3394 | 1/1   | 0.91 | 0.62 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | QA    | 1705 | 1/1   | 0.92 | 0.24 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3042 | 1/1   | 0.98 | 0.24 | -    | 7,7,7,7                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3257 | 1/1   | 0.94 | 0.24 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | YB    | 203  | 1/1   | 0.92 | 0.33 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3188 | 1/1   | 0.78 | 0.25 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3160 | 1/1   | 0.96 | 0.27 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | RA    | 3271 | 1/1   | 0.95 | 0.10 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | QA    | 1633 | 1/1   | 0.98 | 0.42 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | RA    | 3109 | 1/1   | 0.97 | 0.62 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3257 | 1/1   | 0.96 | 0.13 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3189 | 1/1   | 0.99 | 0.21 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | XA    | 1649 | 1/1   | 0.99 | 0.14 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | YE    | 301  | 1/1   | 0.98 | 0.15 | -    | 4,4,4,4                     | 0     |
| 56  | MG   | YA    | 3323 | 1/1   | 0.83 | 0.34 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3346 | 1/1   | 0.92 | 0.13 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3023 | 1/1   | 0.84 | 0.39 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3039 | 1/1   | 0.98 | 0.51 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | XA    | 1677 | 1/1   | 0.91 | 0.11 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3281 | 1/1   | 0.91 | 0.13 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3373 | 1/1   | 0.84 | 0.47 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | XA    | 1722 | 1/1   | 0.90 | 0.15 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3405 | 1/1   | 0.83 | 0.41 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3214 | 1/1   | 0.84 | 0.33 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3370 | 1/1   | 0.98 | 0.33 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | XA    | 1756 | 1/1   | 0.86 | 0.25 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | RA    | 3187 | 1/1   | 0.88 | 0.52 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | QA    | 1689 | 1/1   | 0.93 | 0.45 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3375 | 1/1   | 0.94 | 0.32 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | XA    | 1727 | 1/1   | 0.79 | 1.21 | -    | 78,78,78,78                 | 0     |
| 56  | MG   | RA    | 3315 | 1/1   | 0.92 | 0.31 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3395 | 1/1   | 0.77 | 0.20 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3091 | 1/1   | 0.90 | 0.22 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3015 | 1/1   | 0.96 | 0.28 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | RA    | 3307 | 1/1   | 0.75 | 0.32 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3182 | 1/1   | 0.73 | 0.28 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3324 | 1/1   | 0.83 | 0.24 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3057 | 1/1   | 0.99 | 0.33 | -    | 3,3,3,3                     | 0     |
| 56  | MG   | YA    | 3216 | 1/1   | 0.92 | 0.28 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | YA    | 3447 | 1/1   | 0.84 | 0.27 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3125 | 1/1   | 0.97 | 0.22 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | YA    | 3386 | 1/1   | 0.76 | 0.45 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3255 | 1/1   | 0.96 | 0.27 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1641 | 1/1   | 0.94 | 0.16 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3188 | 1/1   | 0.80 | 0.36 | -    | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3304 | 1/1   | 0.86 | 0.19 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | YA    | 3085 | 1/1   | 0.96 | 0.36 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3019 | 1/1   | 0.92 | 0.36 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | XA    | 1705 | 1/1   | 0.89 | 0.63 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3379 | 1/1   | 0.92 | 0.23 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3117 | 1/1   | 0.93 | 0.35 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | RA    | 3117 | 1/1   | 0.94 | 0.31 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | QA    | 1694 | 1/1   | 0.92 | 0.22 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | XA    | 1670 | 1/1   | 0.90 | 0.33 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3087 | 1/1   | 0.98 | 0.20 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3245 | 1/1   | 0.90 | 0.31 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3299 | 1/1   | 0.51 | 0.44 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3270 | 1/1   | 0.88 | 0.27 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3422 | 1/1   | 0.74 | 0.29 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3219 | 1/1   | 0.96 | 0.16 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | YA    | 3273 | 1/1   | 0.97 | 0.18 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3246 | 1/1   | 0.92 | 0.44 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3421 | 1/1   | 0.86 | 0.21 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | YA    | 3243 | 1/1   | 0.95 | 0.18 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3178 | 1/1   | 0.93 | 0.17 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | QA    | 1630 | 1/1   | 0.75 | 0.33 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3327 | 1/1   | 0.96 | 0.12 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | XA    | 1749 | 1/1   | 0.92 | 0.22 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3251 | 1/1   | 0.93 | 0.16 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3069 | 1/1   | 0.90 | 0.18 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3043 | 1/1   | 0.97 | 0.24 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | YA    | 3368 | 1/1   | 0.89 | 0.18 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | R2    | 101  | 1/1   | 0.89 | 0.25 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | XA    | 1676 | 1/1   | 0.96 | 0.15 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3416 | 1/1   | 0.85 | 0.72 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | QA    | 1610 | 1/1   | 0.95 | 0.12 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | QX    | 101  | 1/1   | 0.97 | 0.23 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3362 | 1/1   | 0.86 | 0.42 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3305 | 1/1   | 0.76 | 0.35 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3191 | 1/1   | 0.81 | 0.15 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | RA    | 3220 | 1/1   | 0.58 | 0.47 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | YA    | 3366 | 1/1   | 0.83 | 0.19 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3154 | 1/1   | 0.95 | 0.15 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | YA    | 3438 | 1/1   | 0.86 | 0.22 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3371 | 1/1   | 0.94 | 0.40 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3409 | 1/1   | 0.99 | 0.39 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | YA    | 3475 | 1/1   | 0.96 | 0.17 | -    | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3190 | 1/1   | 0.92 | 0.37 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3334 | 1/1   | 0.89 | 0.87 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3029 | 1/1   | 0.96 | 0.24 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | RA    | 3008 | 1/1   | 0.95 | 0.96 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | RA    | 3212 | 1/1   | 0.95 | 0.34 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | QA    | 1623 | 1/1   | 0.92 | 0.74 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | R0    | 103  | 1/1   | 0.98 | 0.19 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | QA    | 1646 | 1/1   | 0.93 | 0.37 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | XA    | 1608 | 1/1   | 0.93 | 0.44 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3403 | 1/1   | 0.94 | 0.29 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3277 | 1/1   | 0.69 | 0.51 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3113 | 1/1   | 0.97 | 0.11 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | RA    | 3419 | 1/1   | 0.97 | 0.10 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3367 | 1/1   | 0.96 | 0.29 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3075 | 1/1   | 0.42 | 0.46 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | RB    | 202  | 1/1   | 0.93 | 0.35 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3340 | 1/1   | 0.86 | 0.43 | -    | 72,72,72,72                 | 0     |
| 56  | MG   | Y7    | 101  | 1/1   | 0.68 | 0.40 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3142 | 1/1   | 0.94 | 0.32 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3119 | 1/1   | 0.96 | 0.15 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | YA    | 3441 | 1/1   | 0.85 | 0.18 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3290 | 1/1   | 0.83 | 0.31 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3267 | 1/1   | 0.90 | 0.21 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | QA    | 1747 | 1/1   | 0.62 | 0.37 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | XA    | 1710 | 1/1   | 0.88 | 0.28 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3271 | 1/1   | 0.89 | 0.17 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3313 | 1/1   | 0.93 | 0.42 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | YA    | 3063 | 1/1   | 0.96 | 0.18 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | QA    | 1665 | 1/1   | 0.79 | 0.14 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | XA    | 1616 | 1/1   | 0.97 | 0.25 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | QA    | 1697 | 1/1   | 0.93 | 0.53 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3014 | 1/1   | 0.94 | 0.31 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | YA    | 3145 | 1/1   | 0.92 | 0.13 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | YA    | 3427 | 1/1   | 0.90 | 0.26 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3385 | 1/1   | 0.92 | 0.40 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3288 | 1/1   | 0.74 | 0.26 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3412 | 1/1   | 0.86 | 0.37 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3262 | 1/1   | 0.92 | 0.33 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3219 | 1/1   | 0.92 | 0.31 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | YA    | 3285 | 1/1   | 0.81 | 0.36 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3435 | 1/1   | 0.98 | 0.07 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | QA    | 1713 | 1/1   | 0.92 | 0.28 | -    | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | XA    | 1694 | 1/1   | 0.96 | 0.14 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3383 | 1/1   | 0.86 | 0.26 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3253 | 1/1   | 0.78 | 0.59 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | XA    | 1696 | 1/1   | 0.61 | 0.34 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | QA    | 1734 | 1/1   | 0.65 | 0.41 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3015 | 1/1   | 0.96 | 0.27 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | YA    | 3315 | 1/1   | 0.80 | 0.39 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3093 | 1/1   | 0.85 | 0.11 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3120 | 1/1   | 0.96 | 0.54 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | XA    | 1746 | 1/1   | 0.92 | 0.15 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | XA    | 1703 | 1/1   | 0.94 | 0.39 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3047 | 1/1   | 0.91 | 0.42 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | RA    | 3210 | 1/1   | 0.94 | 0.50 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3076 | 1/1   | 0.98 | 0.17 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3333 | 1/1   | 0.85 | 0.36 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3147 | 1/1   | 0.89 | 0.21 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | QA    | 1704 | 1/1   | 0.96 | 0.56 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3297 | 1/1   | 0.95 | 0.45 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | QA    | 1642 | 1/1   | 0.97 | 0.14 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | XA    | 1685 | 1/1   | 0.93 | 0.50 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3096 | 1/1   | 0.96 | 0.30 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3393 | 1/1   | 0.92 | 0.49 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | YA    | 3065 | 1/1   | 0.95 | 0.24 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3328 | 1/1   | 0.86 | 0.46 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3371 | 1/1   | 0.87 | 0.60 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | RA    | 3297 | 1/1   | 0.95 | 0.34 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3031 | 1/1   | 0.95 | 0.33 | -    | 6,6,6,6                     | 0     |
| 56  | MG   | QA    | 1647 | 1/1   | 0.74 | 0.27 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3176 | 1/1   | 0.95 | 0.40 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | Y5    | 102  | 1/1   | 0.57 | 0.55 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3136 | 1/1   | 0.93 | 0.34 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3172 | 1/1   | 0.88 | 0.13 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3306 | 1/1   | 0.99 | 0.20 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3112 | 1/1   | 0.95 | 0.14 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | RA    | 3134 | 1/1   | 0.50 | 0.79 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1686 | 1/1   | 0.91 | 1.10 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3265 | 1/1   | 0.91 | 0.26 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3062 | 1/1   | 0.99 | 0.35 | -    | 5,5,5,5                     | 0     |
| 56  | MG   | YA    | 3252 | 1/1   | 0.94 | 0.50 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3105 | 1/1   | 0.91 | 0.21 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3323 | 1/1   | 0.94 | 0.07 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3404 | 1/1   | 0.95 | 0.39 | -    | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3344 | 1/1   | 0.96 | 0.13 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | RA    | 3151 | 1/1   | 0.83 | 0.35 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | YV    | 201  | 1/1   | 0.89 | 0.29 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | QA    | 1698 | 1/1   | 0.94 | 0.13 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3216 | 1/1   | 0.95 | 0.32 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | RA    | 3252 | 1/1   | 0.89 | 0.26 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | YA    | 3180 | 1/1   | 0.94 | 0.23 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3395 | 1/1   | 0.97 | 0.40 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3410 | 1/1   | 0.92 | 0.11 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3384 | 1/1   | 0.78 | 0.40 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3282 | 1/1   | 0.95 | 0.07 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3229 | 1/1   | 0.86 | 0.49 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | QA    | 1710 | 1/1   | 0.88 | 0.32 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | XA    | 1651 | 1/1   | 0.95 | 0.21 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | QA    | 1723 | 1/1   | 0.98 | 0.66 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3098 | 1/1   | 0.90 | 0.23 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3232 | 1/1   | 0.80 | 0.25 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3114 | 1/1   | 0.94 | 0.20 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | RA    | 3118 | 1/1   | 0.98 | 0.32 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3285 | 1/1   | 0.91 | 0.32 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3142 | 1/1   | 0.96 | 0.23 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | RA    | 3224 | 1/1   | 0.94 | 0.19 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | XA    | 1747 | 1/1   | 0.90 | 0.12 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3247 | 1/1   | 0.94 | 0.29 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3378 | 1/1   | 0.74 | 0.28 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3396 | 1/1   | 0.91 | 0.24 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3227 | 1/1   | 0.94 | 0.12 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3158 | 1/1   | 0.79 | 0.28 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | YA    | 3382 | 1/1   | 0.94 | 0.40 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3048 | 1/1   | 0.90 | 0.28 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3134 | 1/1   | 0.98 | 0.33 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3351 | 1/1   | 0.86 | 0.24 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | QA    | 1607 | 1/1   | 0.98 | 0.28 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | QA    | 1652 | 1/1   | 0.91 | 0.19 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3261 | 1/1   | 0.93 | 0.22 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3041 | 1/1   | 0.89 | 0.26 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | RA    | 3246 | 1/1   | 0.92 | 0.24 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3478 | 1/1   | 0.86 | 0.15 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | XA    | 1626 | 1/1   | 0.96 | 0.34 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3150 | 1/1   | 0.90 | 0.40 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | RA    | 3302 | 1/1   | 0.92 | 0.14 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3096 | 1/1   | 0.82 | 0.10 | -    | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | XA    | 1654 | 1/1   | 0.89 | 0.49 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3226 | 1/1   | 0.91 | 0.19 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | QA    | 1677 | 1/1   | 0.81 | 0.12 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | XA    | 1735 | 1/1   | 0.97 | 0.26 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | XA    | 1619 | 1/1   | 0.98 | 0.15 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | RA    | 3020 | 1/1   | 0.96 | 0.30 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | YA    | 3307 | 1/1   | 0.86 | 0.34 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3086 | 1/1   | 0.96 | 0.25 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | RA    | 3146 | 1/1   | 0.82 | 0.21 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3270 | 1/1   | 0.96 | 0.33 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3010 | 1/1   | 0.97 | 0.41 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | XA    | 1639 | 1/1   | 0.97 | 0.39 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3097 | 1/1   | 0.91 | 0.31 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | QA    | 1674 | 1/1   | 0.93 | 0.55 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3169 | 1/1   | 0.89 | 0.31 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3389 | 1/1   | 0.85 | 0.17 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3124 | 1/1   | 0.97 | 0.23 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | XA    | 1684 | 1/1   | 0.92 | 0.14 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3276 | 1/1   | 0.85 | 0.25 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | XA    | 1699 | 1/1   | 0.98 | 0.17 | -    | 78,78,78,78                 | 0     |
| 56  | MG   | QA    | 1621 | 1/1   | 0.91 | 0.16 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3185 | 1/1   | 0.81 | 0.50 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3089 | 1/1   | 0.97 | 0.51 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | RA    | 3406 | 1/1   | 0.77 | 0.52 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | YA    | 3279 | 1/1   | 0.92 | 0.13 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | XA    | 1714 | 1/1   | 0.84 | 0.29 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3390 | 1/1   | 0.85 | 0.16 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | XA    | 1680 | 1/1   | 0.94 | 0.22 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | RA    | 3356 | 1/1   | 0.84 | 0.10 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3215 | 1/1   | 0.88 | 0.39 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | XA    | 1724 | 1/1   | 0.83 | 0.20 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | YW    | 201  | 1/1   | 0.93 | 0.53 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3245 | 1/1   | 0.73 | 0.18 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3391 | 1/1   | 0.58 | 0.43 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | QA    | 1635 | 1/1   | 0.97 | 0.40 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3300 | 1/1   | 0.73 | 0.26 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3429 | 1/1   | 0.94 | 0.25 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3464 | 1/1   | 0.87 | 0.17 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | XA    | 1737 | 1/1   | 0.94 | 0.47 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | XA    | 1758 | 1/1   | 0.81 | 0.76 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | RV    | 201  | 1/1   | 0.89 | 0.33 | -    | 4,4,4,4                     | 0     |
| 56  | MG   | RA    | 3236 | 1/1   | 0.94 | 0.43 | -    | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3291 | 1/1   | 0.93 | 0.28 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | XA    | 1657 | 1/1   | 0.97 | 0.23 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3430 | 1/1   | 0.91 | 0.17 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3044 | 1/1   | 0.96 | 0.32 | -    | 1,1,1,1                     | 0     |
| 56  | MG   | RA    | 3336 | 1/1   | 0.83 | 0.14 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3036 | 1/1   | 0.97 | 0.38 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | XA    | 1728 | 1/1   | 0.88 | 0.57 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3335 | 1/1   | 0.94 | 0.34 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3324 | 1/1   | 0.85 | 0.30 | -    | 75,75,75,75                 | 0     |
| 56  | MG   | YA    | 3374 | 1/1   | 0.96 | 0.18 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3185 | 1/1   | 0.91 | 0.19 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | QA    | 1695 | 1/1   | 0.81 | 0.54 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3266 | 1/1   | 0.93 | 0.46 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3268 | 1/1   | 0.82 | 0.58 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3139 | 1/1   | 0.97 | 0.17 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3239 | 1/1   | 0.89 | 0.58 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3283 | 1/1   | 0.73 | 0.14 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | XA    | 1655 | 1/1   | 0.95 | 0.18 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3359 | 1/1   | 0.95 | 0.16 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | RA    | 3054 | 1/1   | 0.95 | 0.36 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | YA    | 3159 | 1/1   | 0.93 | 0.27 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3453 | 1/1   | 0.84 | 0.19 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3364 | 1/1   | 0.88 | 0.27 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | QA    | 1746 | 1/1   | 0.61 | 0.49 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | YA    | 3403 | 1/1   | 0.87 | 0.19 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3171 | 1/1   | 0.52 | 0.40 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3347 | 1/1   | 0.71 | 0.74 | -    | 83,83,83,83                 | 0     |
| 56  | MG   | YA    | 3110 | 1/1   | 0.88 | 0.14 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3280 | 1/1   | 0.99 | 0.25 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3278 | 1/1   | 0.82 | 0.46 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | QA    | 1653 | 1/1   | 0.98 | 0.14 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | QA    | 1731 | 1/1   | 0.79 | 0.13 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3362 | 1/1   | 0.91 | 0.09 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3322 | 1/1   | 0.53 | 0.45 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3384 | 1/1   | 0.99 | 0.09 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | YA    | 3353 | 1/1   | 0.95 | 0.38 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | RA    | 3397 | 1/1   | 0.82 | 0.22 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3423 | 1/1   | 0.99 | 0.25 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3345 | 1/1   | 0.83 | 0.42 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3391 | 1/1   | 0.90 | 0.35 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | QA    | 1708 | 1/1   | 0.92 | 0.60 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | QA    | 1684 | 1/1   | 0.98 | 0.25 | -    | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3200 | 1/1   | 0.96 | 0.46 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | XA    | 1740 | 1/1   | 0.96 | 0.32 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3167 | 1/1   | 0.92 | 0.21 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3289 | 1/1   | 0.98 | 0.26 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | RA    | 3168 | 1/1   | 0.45 | 0.72 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3232 | 1/1   | 0.87 | 0.37 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3106 | 1/1   | 0.94 | 0.20 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3437 | 1/1   | 0.82 | 0.58 | -    | 89,89,89,89                 | 0     |
| 56  | MG   | YA    | 3357 | 1/1   | 0.45 | 0.74 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3381 | 1/1   | 0.88 | 0.27 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | QA    | 1629 | 1/1   | 0.89 | 0.46 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | QA    | 1660 | 1/1   | 0.98 | 0.19 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3360 | 1/1   | 0.84 | 0.33 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3260 | 1/1   | 0.81 | 0.27 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3317 | 1/1   | 0.76 | 0.56 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3205 | 1/1   | 0.91 | 0.46 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | XA    | 1729 | 1/1   | 0.91 | 0.34 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | QA    | 1622 | 1/1   | 0.94 | 0.23 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3086 | 1/1   | 0.94 | 0.18 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | QA    | 1617 | 1/1   | 0.95 | 0.17 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3177 | 1/1   | 0.94 | 0.35 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | XA    | 1718 | 1/1   | 0.92 | 0.18 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3166 | 1/1   | 0.92 | 0.40 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | QA    | 1618 | 1/1   | 0.93 | 0.26 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | XA    | 1702 | 1/1   | 0.85 | 0.66 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | RT    | 201  | 1/1   | 0.95 | 0.13 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | QA    | 1733 | 1/1   | 0.81 | 0.29 | -    | 86,86,86,86                 | 0     |
| 56  | MG   | RA    | 3293 | 1/1   | 0.97 | 0.39 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3379 | 1/1   | 0.46 | 0.57 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | XA    | 1629 | 1/1   | 0.86 | 0.25 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3292 | 1/1   | 0.86 | 0.49 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | XA    | 1698 | 1/1   | 0.94 | 0.11 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | QA    | 1716 | 1/1   | 0.90 | 0.21 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | RA    | 3249 | 1/1   | 0.73 | 0.24 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | XA    | 1726 | 1/1   | 0.86 | 0.99 | -    | 59,59,59,59                 | 0     |
| 56  | MG   | R1    | 101  | 1/1   | 0.91 | 0.42 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3329 | 1/1   | 0.91 | 0.20 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3401 | 1/1   | 0.84 | 0.19 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | QV    | 102  | 1/1   | 0.90 | 0.26 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3095 | 1/1   | 0.87 | 0.45 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3414 | 1/1   | 0.91 | 0.30 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | R0    | 102  | 1/1   | 0.95 | 0.61 | -    | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3293 | 1/1   | 0.79 | 0.41 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | QD    | 302  | 1/1   | 0.93 | 0.29 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | QA    | 1736 | 1/1   | 0.96 | 0.19 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | RA    | 3123 | 1/1   | 0.94 | 0.43 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3144 | 1/1   | 0.95 | 0.21 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | XA    | 1730 | 1/1   | 0.82 | 0.78 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3248 | 1/1   | 0.94 | 0.37 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3229 | 1/1   | 0.82 | 0.10 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | XA    | 1733 | 1/1   | 0.70 | 0.17 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | XA    | 1713 | 1/1   | 0.83 | 0.14 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | XV    | 103  | 1/1   | 0.89 | 0.32 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3077 | 1/1   | 0.98 | 0.35 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | RA    | 3286 | 1/1   | 0.94 | 0.33 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | YA    | 3242 | 1/1   | 0.90 | 0.53 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3181 | 1/1   | 0.97 | 0.17 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3187 | 1/1   | 0.89 | 0.32 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3202 | 1/1   | 0.97 | 0.26 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | YA    | 3068 | 1/1   | 0.71 | 0.46 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3468 | 1/1   | 0.97 | 0.76 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | XA    | 1751 | 1/1   | 0.92 | 0.31 | -    | 70,70,70,70                 | 0     |
| 56  | MG   | RA    | 3428 | 1/1   | 0.91 | 0.19 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3135 | 1/1   | 0.98 | 0.20 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | RA    | 3342 | 1/1   | 0.50 | 0.47 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | YA    | 3020 | 1/1   | 0.98 | 0.22 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3250 | 1/1   | 0.90 | 0.23 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3345 | 1/1   | 0.59 | 0.31 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3181 | 1/1   | 0.92 | 0.35 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3398 | 1/1   | 0.79 | 0.28 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | YA    | 3157 | 1/1   | 0.86 | 0.34 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | QA    | 1720 | 1/1   | 0.81 | 0.28 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | QA    | 1715 | 1/1   | 0.97 | 0.38 | -    | 72,72,72,72                 | 0     |
| 56  | MG   | RA    | 3294 | 1/1   | 0.95 | 0.12 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | XV    | 102  | 1/1   | 0.92 | 0.22 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3182 | 1/1   | 0.86 | 0.34 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3201 | 1/1   | 0.95 | 0.07 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | XA    | 1720 | 1/1   | 0.98 | 0.17 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | QA    | 1612 | 1/1   | 0.93 | 0.23 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | RA    | 3231 | 1/1   | 0.97 | 0.15 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | YA    | 3337 | 1/1   | 0.95 | 0.14 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3301 | 1/1   | 0.85 | 0.26 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3274 | 1/1   | 0.72 | 0.31 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3143 | 1/1   | 0.92 | 0.14 | -    | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3360 | 1/1   | 0.60 | 0.51 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3053 | 1/1   | 0.97 | 0.49 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3217 | 1/1   | 0.96 | 0.28 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | RA    | 3124 | 1/1   | 0.96 | 0.24 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3115 | 1/1   | 0.97 | 0.31 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3417 | 1/1   | 0.95 | 0.47 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3400 | 1/1   | 0.87 | 0.10 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3034 | 1/1   | 0.98 | 0.33 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | YA    | 3476 | 1/1   | 0.89 | 0.21 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3023 | 1/1   | 0.99 | 0.44 | -    | 2,2,2,2                     | 0     |
| 56  | MG   | QA    | 1701 | 1/1   | 0.74 | 0.18 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | XA    | 1602 | 1/1   | 0.97 | 0.44 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | YA    | 3211 | 1/1   | 0.92 | 0.19 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3043 | 1/1   | 0.95 | 0.35 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3361 | 1/1   | 0.61 | 0.52 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | YA    | 3326 | 1/1   | 0.92 | 0.60 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3393 | 1/1   | 0.95 | 0.21 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1647 | 1/1   | 0.94 | 0.20 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3256 | 1/1   | 0.91 | 0.17 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | RA    | 3230 | 1/1   | 0.90 | 0.43 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | RA    | 3426 | 1/1   | 0.68 | 0.93 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | YA    | 3061 | 1/1   | 0.98 | 0.37 | -    | 0,0,0,0                     | 0     |
| 56  | MG   | XA    | 1687 | 1/1   | 0.89 | 0.26 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3119 | 1/1   | 0.96 | 0.17 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | QA    | 1739 | 1/1   | 0.94 | 0.44 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3140 | 1/1   | 0.83 | 0.21 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3311 | 1/1   | 0.93 | 0.63 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | XA    | 1712 | 1/1   | 0.98 | 0.33 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3409 | 1/1   | 0.96 | 0.21 | -    | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3344 | 1/1   | 0.72 | 0.51 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | YA    | 3469 | 1/1   | 0.94 | 0.20 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | RA    | 3354 | 1/1   | 0.88 | 0.31 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | QA    | 1683 | 1/1   | 0.84 | 0.50 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3480 | 1/1   | 0.83 | 0.15 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | YA    | 3452 | 1/1   | 0.86 | 0.17 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3024 | 1/1   | 0.98 | 0.28 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | YA    | 3207 | 1/1   | 0.98 | 0.19 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | YB    | 202  | 1/1   | 0.85 | 0.27 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3137 | 1/1   | 0.92 | 0.18 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3045 | 1/1   | 0.95 | 0.23 | -    | 3,3,3,3                     | 0     |
| 56  | MG   | YA    | 3235 | 1/1   | 0.91 | 0.63 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3487 | 1/1   | 0.97 | 0.34 | -    | 18,18,18,18                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3076 | 1/1   | 0.94 | 0.38 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | YA    | 3272 | 1/1   | 0.93 | 0.26 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3035 | 1/1   | 0.99 | 0.16 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | XA    | 1752 | 1/1   | 0.97 | 0.14 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3038 | 1/1   | 0.98 | 0.23 | -    | 2,2,2,2                     | 0     |
| 56  | MG   | XA    | 1725 | 1/1   | 0.85 | 0.31 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3028 | 1/1   | 0.96 | 0.27 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | QA    | 1634 | 1/1   | 0.86 | 0.20 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3116 | 1/1   | 0.95 | 0.27 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | YA    | 3477 | 1/1   | 0.94 | 0.35 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3052 | 1/1   | 0.97 | 0.30 | -    | 1,1,1,1                     | 0     |
| 56  | MG   | RA    | 3333 | 1/1   | 0.90 | 0.30 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3208 | 1/1   | 0.96 | 0.30 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3389 | 1/1   | 0.90 | 0.10 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3173 | 1/1   | 0.89 | 0.39 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3272 | 1/1   | 0.93 | 0.12 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3068 | 1/1   | 0.95 | 0.40 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | RA    | 3199 | 1/1   | 0.84 | 0.65 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3122 | 1/1   | 0.97 | 0.39 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | XA    | 1678 | 1/1   | 0.92 | 0.34 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3338 | 1/1   | 0.68 | 0.43 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | RA    | 3241 | 1/1   | 0.93 | 0.31 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3003 | 1/1   | 0.99 | 0.26 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | YA    | 3376 | 1/1   | 0.83 | 0.20 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3380 | 1/1   | 0.86 | 0.41 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3196 | 1/1   | 0.67 | 0.27 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | XA    | 1738 | 1/1   | 0.78 | 0.18 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3256 | 1/1   | 0.85 | 0.41 | -    | 93,93,93,93                 | 0     |
| 56  | MG   | XA    | 1673 | 1/1   | 0.96 | 0.10 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3277 | 1/1   | 0.90 | 0.31 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | RA    | 3183 | 1/1   | 0.94 | 0.23 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | RA    | 3392 | 1/1   | 0.82 | 0.28 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | RA    | 3046 | 1/1   | 0.97 | 0.44 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | YA    | 3350 | 1/1   | 0.90 | 0.15 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3162 | 1/1   | 0.84 | 0.45 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3449 | 1/1   | 0.93 | 0.47 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | QA    | 1672 | 1/1   | 0.95 | 0.65 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | RA    | 3317 | 1/1   | 0.95 | 0.22 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1743 | 1/1   | 0.85 | 0.10 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3051 | 1/1   | 0.85 | 0.69 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3254 | 1/1   | 0.95 | 0.40 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3242 | 1/1   | 0.96 | 0.08 | -    | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3100 | 1/1   | 0.83 | 0.30 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | XA    | 1744 | 1/1   | 0.85 | 0.61 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | YA    | 3290 | 1/1   | 0.68 | 0.37 | -    | 82,82,82,82                 | 0     |
| 56  | MG   | RA    | 3374 | 1/1   | 0.96 | 0.32 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3036 | 1/1   | 0.96 | 0.30 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3193 | 1/1   | 0.94 | 0.17 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3194 | 1/1   | 0.97 | 0.38 | -    | 21,21,21,21                 | 0     |
| 56  | MG   | RA    | 3049 | 1/1   | 0.95 | 0.37 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3269 | 1/1   | 0.93 | 0.33 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3309 | 1/1   | 0.96 | 0.74 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3126 | 1/1   | 0.98 | 0.27 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | QA    | 1707 | 1/1   | 0.85 | 0.61 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3194 | 1/1   | 0.97 | 0.28 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | QA    | 1648 | 1/1   | 0.90 | 0.12 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3304 | 1/1   | 0.95 | 0.35 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3415 | 1/1   | 0.90 | 0.18 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | YY    | 201  | 1/1   | 0.94 | 0.20 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3217 | 1/1   | 0.98 | 0.19 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | YA    | 3197 | 1/1   | 0.96 | 0.38 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3423 | 1/1   | 0.89 | 0.38 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | QA    | 1650 | 1/1   | 0.88 | 0.44 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | Y0    | 103  | 1/1   | 0.87 | 0.33 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | QA    | 1692 | 1/1   | 0.81 | 0.45 | -    | 65,65,65,65                 | 0     |
| 56  | MG   | XA    | 1621 | 1/1   | 0.86 | 0.22 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3174 | 1/1   | 0.98 | 0.15 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | XL    | 201  | 1/1   | 0.84 | 0.17 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | XA    | 1660 | 1/1   | 0.95 | 0.38 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3287 | 1/1   | 0.83 | 0.36 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3343 | 1/1   | 0.90 | 0.21 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3412 | 1/1   | 0.87 | 0.16 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | XA    | 1693 | 1/1   | 0.83 | 0.14 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | RA    | 3330 | 1/1   | 0.94 | 0.15 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3223 | 1/1   | 0.95 | 0.25 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3078 | 1/1   | 0.97 | 0.41 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | XA    | 1759 | 1/1   | 0.72 | 0.66 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3199 | 1/1   | 0.91 | 0.29 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | QA    | 1700 | 1/1   | 0.97 | 0.56 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3418 | 1/1   | 0.92 | 0.35 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3098 | 1/1   | 0.94 | 0.38 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3077 | 1/1   | 0.97 | 0.42 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | XA    | 1681 | 1/1   | 0.97 | 0.35 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | RA    | 3130 | 1/1   | 0.98 | 0.29 | -    | 12,12,12,12                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3387 | 1/1   | 0.97 | 0.42 | -    | 16,16,16,16                 | 0     |
| 56  | MG   | YA    | 3129 | 1/1   | 0.93 | 0.35 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | YB    | 204  | 1/1   | 0.92 | 0.09 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | QA    | 1657 | 1/1   | 0.98 | 0.17 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | QA    | 1732 | 1/1   | 0.94 | 0.08 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | XA    | 1688 | 1/1   | 0.84 | 0.59 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3094 | 1/1   | 0.91 | 0.08 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3381 | 1/1   | 0.98 | 0.46 | -    | 0,0,0,0                     | 0     |
| 56  | MG   | YA    | 3332 | 1/1   | 0.90 | 0.47 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3001 | 1/1   | 0.70 | 0.94 | -    | 73,73,73,73                 | 0     |
| 56  | MG   | Y5    | 101  | 1/1   | 0.97 | 0.17 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | QA    | 1631 | 1/1   | 0.95 | 0.38 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | XA    | 1661 | 1/1   | 0.97 | 0.30 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3481 | 1/1   | 0.90 | 0.50 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3319 | 1/1   | 0.94 | 0.14 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3388 | 1/1   | 0.96 | 0.47 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | RA    | 3402 | 1/1   | 0.87 | 0.53 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | XA    | 1716 | 1/1   | 0.98 | 0.37 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | RA    | 3019 | 1/1   | 0.98 | 0.27 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | RA    | 3383 | 1/1   | 0.91 | 0.78 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | XA    | 1709 | 1/1   | 0.99 | 0.50 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | RA    | 3287 | 1/1   | 0.97 | 0.09 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3258 | 1/1   | 0.93 | 0.09 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | XA    | 1711 | 1/1   | 0.91 | 0.45 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3312 | 1/1   | 0.92 | 0.49 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3361 | 1/1   | 0.96 | 0.55 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | XA    | 1674 | 1/1   | 0.96 | 0.24 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | RA    | 3058 | 1/1   | 0.99 | 0.29 | -    | 1,1,1,1                     | 0     |
| 56  | MG   | QA    | 1690 | 1/1   | 0.98 | 0.09 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3234 | 1/1   | 0.96 | 0.15 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3479 | 1/1   | 0.92 | 0.13 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3309 | 1/1   | 0.91 | 0.16 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3303 | 1/1   | 0.89 | 0.24 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3299 | 1/1   | 0.96 | 0.29 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3148 | 1/1   | 0.98 | 0.31 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3118 | 1/1   | 0.88 | 0.34 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | QA    | 1658 | 1/1   | 0.94 | 0.91 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3465 | 1/1   | 0.95 | 0.09 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | RA    | 3400 | 1/1   | 0.90 | 0.24 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3483 | 1/1   | 0.96 | 0.96 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | RA    | 3089 | 1/1   | 0.91 | 0.29 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | QA    | 1661 | 1/1   | 0.94 | 0.12 | -    | 23,23,23,23                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3278 | 1/1   | 0.95 | 0.42 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3213 | 1/1   | 0.94 | 0.38 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | QA    | 1638 | 1/1   | 0.94 | 0.39 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | RA    | 3308 | 1/1   | 0.94 | 0.28 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | XA    | 1606 | 1/1   | 0.99 | 0.29 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3404 | 1/1   | 0.99 | 0.35 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | XA    | 1739 | 1/1   | 0.84 | 0.26 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | XA    | 1610 | 1/1   | 0.98 | 0.22 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | YA    | 3230 | 1/1   | 0.97 | 0.32 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1668 | 1/1   | 0.98 | 0.44 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | RA    | 3114 | 1/1   | 0.61 | 0.31 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | XA    | 1637 | 1/1   | 0.94 | 0.17 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | XA    | 1715 | 1/1   | 0.87 | 0.43 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3092 | 1/1   | 0.87 | 0.45 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | XA    | 1631 | 1/1   | 0.93 | 0.36 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | XA    | 1622 | 1/1   | 0.90 | 0.76 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3349 | 1/1   | 0.86 | 0.60 | -    | 55,55,55,55                 | 0     |
| 56  | MG   | RA    | 3192 | 1/1   | 0.99 | 0.47 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | YA    | 3310 | 1/1   | 0.94 | 0.44 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3090 | 1/1   | 0.96 | 0.42 | -    | 4,4,4,4                     | 0     |
| 56  | MG   | YA    | 3169 | 1/1   | 0.88 | 0.25 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | YA    | 3179 | 1/1   | 0.94 | 0.40 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | QA    | 1722 | 1/1   | 0.86 | 0.14 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | RA    | 3301 | 1/1   | 0.96 | 0.18 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3198 | 1/1   | 0.94 | 0.27 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | RA    | 3352 | 1/1   | 0.81 | 0.48 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | QA    | 1745 | 1/1   | 0.81 | 0.27 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | RA    | 3262 | 1/1   | 0.95 | 0.12 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | YA    | 3433 | 1/1   | 0.93 | 0.20 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | RA    | 3211 | 1/1   | 0.86 | 0.14 | -    | 11,11,11,11                 | 0     |
| 56  | MG   | RA    | 3258 | 1/1   | 0.86 | 0.33 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | XA    | 1612 | 1/1   | 0.94 | 0.14 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | YH    | 201  | 1/1   | 0.15 | 0.61 | -    | 118,118,118,118             | 0     |
| 56  | MG   | YA    | 3139 | 1/1   | 0.96 | 0.28 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | RA    | 3320 | 1/1   | 0.73 | 0.62 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3143 | 1/1   | 0.96 | 0.19 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3377 | 1/1   | 0.95 | 0.22 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3037 | 1/1   | 0.99 | 0.36 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | XA    | 1628 | 1/1   | 0.97 | 0.49 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3296 | 1/1   | 0.91 | 0.23 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3180 | 1/1   | 0.88 | 0.26 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | RA    | 3410 | 1/1   | 0.91 | 0.36 | -    | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3107 | 1/1   | 0.94 | 0.42 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | RA    | 3413 | 1/1   | 0.75 | 0.38 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | XA    | 1636 | 1/1   | 0.94 | 0.26 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | YA    | 3007 | 1/1   | 0.96 | 1.05 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3396 | 1/1   | 0.68 | 0.27 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | XA    | 1662 | 1/1   | 0.90 | 0.28 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3358 | 1/1   | 0.92 | 0.33 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | XA    | 1757 | 1/1   | 0.84 | 0.61 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | YA    | 3163 | 1/1   | 0.63 | 0.55 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3419 | 1/1   | 0.98 | 0.23 | -    | 2,2,2,2                     | 0     |
| 56  | MG   | XA    | 1721 | 1/1   | 0.87 | 0.21 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3348 | 1/1   | 0.94 | 0.23 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | XA    | 1671 | 1/1   | 0.96 | 0.11 | -    | 0,0,0,0                     | 0     |
| 56  | MG   | RA    | 3433 | 1/1   | 0.92 | 0.22 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | QA    | 1664 | 1/1   | 0.98 | 0.21 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3067 | 1/1   | 0.98 | 0.38 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3313 | 1/1   | 0.85 | 0.48 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | RA    | 3160 | 1/1   | 0.94 | 0.39 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3222 | 1/1   | 0.92 | 0.35 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3149 | 1/1   | 0.78 | 0.40 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | YA    | 3436 | 1/1   | 0.80 | 0.58 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3186 | 1/1   | 0.81 | 0.19 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | XA    | 1632 | 1/1   | 0.94 | 0.27 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3196 | 1/1   | 0.95 | 0.39 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3408 | 1/1   | 0.87 | 0.44 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | XA    | 1665 | 1/1   | 0.93 | 0.40 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3156 | 1/1   | 0.94 | 0.09 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3115 | 1/1   | 0.95 | 0.36 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | XA    | 1704 | 1/1   | 0.91 | 0.13 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3153 | 1/1   | 0.71 | 0.40 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | XA    | 1646 | 1/1   | 0.84 | 0.49 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3432 | 1/1   | 0.69 | 0.58 | -    | 78,78,78,78                 | 0     |
| 56  | MG   | YA    | 3266 | 1/1   | 0.95 | 0.25 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3363 | 1/1   | 0.87 | 0.52 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | XA    | 1707 | 1/1   | 0.94 | 0.67 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | QA    | 1669 | 1/1   | 0.77 | 0.18 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | YA    | 3330 | 1/1   | 0.91 | 0.23 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | RA    | 3314 | 1/1   | 0.93 | 0.33 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | RA    | 3328 | 1/1   | 0.82 | 0.37 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | YA    | 3329 | 1/1   | 0.85 | 0.48 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | RA    | 3152 | 1/1   | 0.90 | 0.44 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | Y0    | 102  | 1/1   | 0.90 | 0.11 | -    | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3446 | 1/1   | 0.99 | 0.26 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | RA    | 3145 | 1/1   | 0.97 | 0.25 | -    | 9,9,9,9                     | 0     |
| 56  | MG   | RA    | 3322 | 1/1   | 0.93 | 0.12 | -    | 15,15,15,15                 | 0     |
| 56  | MG   | YA    | 3241 | 1/1   | 0.95 | 0.25 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3349 | 1/1   | 0.89 | 0.34 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3231 | 1/1   | 0.83 | 0.20 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3207 | 1/1   | 0.98 | 0.21 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | RA    | 3380 | 1/1   | 0.67 | 0.20 | -    | 61,61,61,61                 | 0     |
| 56  | MG   | YA    | 3141 | 1/1   | 0.89 | 0.26 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | YA    | 3004 | 1/1   | 0.91 | 0.36 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | XA    | 1700 | 1/1   | 0.82 | 0.45 | -    | 79,79,79,79                 | 0     |
| 56  | MG   | RA    | 3064 | 1/1   | 0.99 | 0.23 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | YA    | 3132 | 1/1   | 0.77 | 0.65 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | XA    | 1719 | 1/1   | 0.82 | 0.24 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3021 | 1/1   | 0.97 | 0.21 | -    | 4,4,4,4                     | 0     |
| 56  | MG   | YA    | 3319 | 1/1   | 0.83 | 0.21 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | RA    | 3005 | 1/1   | 0.98 | 0.66 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3022 | 1/1   | 0.95 | 0.53 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | YO    | 201  | 1/1   | 0.83 | 0.24 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3308 | 1/1   | 0.86 | 0.38 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | YA    | 3123 | 1/1   | 0.95 | 0.36 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3120 | 1/1   | 0.84 | 0.89 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3195 | 1/1   | 0.90 | 0.17 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | R0    | 101  | 1/1   | 0.84 | 0.44 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3288 | 1/1   | 0.97 | 0.19 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | QA    | 1680 | 1/1   | 0.86 | 0.31 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | RA    | 3084 | 1/1   | 0.92 | 0.19 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | XA    | 1658 | 1/1   | 0.76 | 0.15 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3372 | 1/1   | 0.95 | 0.20 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | RA    | 3138 | 1/1   | 0.95 | 0.29 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | XA    | 1663 | 1/1   | 0.94 | 0.24 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | XA    | 1666 | 1/1   | 0.91 | 0.26 | -    | 39,39,39,39                 | 0     |
| 56  | MG   | RA    | 3332 | 1/1   | 0.74 | 0.31 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | YA    | 3311 | 1/1   | 0.89 | 0.27 | -    | 74,74,74,74                 | 0     |
| 56  | MG   | YA    | 3408 | 1/1   | 0.82 | 0.14 | -    | 73,73,73,73                 | 0     |
| 56  | MG   | Y0    | 101  | 1/1   | 0.97 | 0.13 | -    | 18,18,18,18                 | 0     |
| 56  | MG   | XA    | 1648 | 1/1   | 0.90 | 0.24 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3415 | 1/1   | 0.49 | 0.52 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | YA    | 3100 | 1/1   | 0.98 | 0.28 | -    | 3,3,3,3                     | 0     |
| 56  | MG   | RA    | 3325 | 1/1   | 0.86 | 0.28 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3083 | 1/1   | 0.89 | 0.24 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3331 | 1/1   | 0.94 | 0.20 | -    | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | QA    | 1620 | 1/1   | 0.95 | 0.15 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | QA    | 1616 | 1/1   | 0.94 | 0.19 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | QA    | 1679 | 1/1   | 0.93 | 0.20 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | QA    | 1718 | 1/1   | 0.93 | 0.34 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3302 | 1/1   | 0.76 | 0.30 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | RA    | 3441 | 1/1   | 0.96 | 0.28 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | RA    | 3126 | 1/1   | 0.95 | 0.20 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3470 | 1/1   | 0.95 | 0.27 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3366 | 1/1   | 0.93 | 0.24 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3274 | 1/1   | 0.98 | 0.41 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3399 | 1/1   | 0.86 | 0.60 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | YA    | 3184 | 1/1   | 0.84 | 0.30 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3352 | 1/1   | 0.92 | 0.13 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | QA    | 1655 | 1/1   | 0.98 | 0.44 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3113 | 1/1   | 0.98 | 0.28 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3300 | 1/1   | 0.97 | 0.33 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | XA    | 1708 | 1/1   | 0.97 | 0.27 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3448 | 1/1   | 0.70 | 0.40 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | QA    | 1714 | 1/1   | 0.98 | 0.13 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | QA    | 1727 | 1/1   | 0.87 | 0.35 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3088 | 1/1   | 0.97 | 0.20 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | RA    | 3417 | 1/1   | 0.57 | 0.36 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | YA    | 3466 | 1/1   | 0.89 | 0.43 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3158 | 1/1   | 0.98 | 0.28 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | QA    | 1696 | 1/1   | 0.75 | 0.91 | -    | 67,67,67,67                 | 0     |
| 56  | MG   | YA    | 3443 | 1/1   | 0.92 | 0.14 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | RA    | 3127 | 1/1   | 0.86 | 0.62 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3152 | 1/1   | 0.65 | 0.33 | -    | 54,54,54,54                 | 0     |
| 56  | MG   | QA    | 1675 | 1/1   | 0.88 | 0.12 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | RA    | 3334 | 1/1   | 0.92 | 0.65 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3102 | 1/1   | 0.73 | 0.34 | -    | 10,10,10,10                 | 0     |
| 56  | MG   | YA    | 3355 | 1/1   | 0.81 | 0.49 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | XA    | 1669 | 1/1   | 0.94 | 0.30 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3002 | 1/1   | 0.95 | 0.15 | -    | 0,0,0,0                     | 0     |
| 56  | MG   | QA    | 1603 | 1/1   | 0.78 | 0.23 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3259 | 1/1   | 0.84 | 0.44 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | XA    | 1675 | 1/1   | 0.81 | 0.91 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | YA    | 3225 | 1/1   | 0.77 | 0.23 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | YA    | 3439 | 1/1   | 0.85 | 0.11 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3178 | 1/1   | 0.96 | 0.21 | -    | 32,32,32,32                 | 0     |
| 56  | MG   | YA    | 3365 | 1/1   | 0.96 | 0.40 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3253 | 1/1   | 0.88 | 0.28 | -    | 19,19,19,19                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | RA    | 3226 | 1/1   | 0.88 | 0.39 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3175 | 1/1   | 0.96 | 0.08 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | RA    | 3218 | 1/1   | 0.95 | 0.21 | -    | 13,13,13,13                 | 0     |
| 56  | MG   | YA    | 3451 | 1/1   | 0.97 | 0.17 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | YA    | 3075 | 1/1   | 0.92 | 0.29 | -    | 8,8,8,8                     | 0     |
| 56  | MG   | RA    | 3025 | 1/1   | 0.98 | 0.21 | -    | 12,12,12,12                 | 0     |
| 56  | MG   | YA    | 3168 | 1/1   | 0.96 | 0.30 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | XA    | 1617 | 1/1   | 0.92 | 0.39 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3382 | 1/1   | 0.95 | 0.27 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3320 | 1/1   | 0.96 | 0.12 | -    | 38,38,38,38                 | 0     |
| 56  | MG   | XA    | 1645 | 1/1   | 0.93 | 0.31 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3358 | 1/1   | 0.90 | 0.16 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | RY    | 201  | 1/1   | 0.75 | 0.43 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | QA    | 1724 | 1/1   | 0.62 | 0.20 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | YA    | 3183 | 1/1   | 0.74 | 0.24 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3040 | 1/1   | 0.97 | 0.47 | -    | 4,4,4,4                     | 0     |
| 56  | MG   | XA    | 1683 | 1/1   | 0.82 | 0.29 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | YA    | 3369 | 1/1   | 0.94 | 0.16 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3265 | 1/1   | 0.83 | 0.23 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | YA    | 3457 | 1/1   | 0.91 | 0.20 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3165 | 1/1   | 0.92 | 0.29 | -    | 34,34,34,34                 | 0     |
| 56  | MG   | YA    | 3422 | 1/1   | 0.73 | 0.14 | -    | 58,58,58,58                 | 0     |
| 56  | MG   | YA    | 3388 | 1/1   | 0.87 | 0.28 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | YA    | 3314 | 1/1   | 0.95 | 0.14 | -    | 47,47,47,47                 | 0     |
| 56  | MG   | RB    | 203  | 1/1   | 0.89 | 0.32 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3359 | 1/1   | 0.93 | 0.15 | -    | 42,42,42,42                 | 0     |
| 56  | MG   | QA    | 1706 | 1/1   | 0.72 | 0.36 | -    | 52,52,52,52                 | 0     |
| 56  | MG   | YA    | 3399 | 1/1   | 0.96 | 0.08 | -    | 57,57,57,57                 | 0     |
| 56  | MG   | RA    | 3112 | 1/1   | 0.98 | 0.08 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | YA    | 3458 | 1/1   | 0.92 | 0.14 | -    | 51,51,51,51                 | 0     |
| 56  | MG   | YA    | 3030 | 1/1   | 0.97 | 0.31 | -    | 3,3,3,3                     | 0     |
| 56  | MG   | YA    | 3144 | 1/1   | 0.93 | 0.17 | -    | 24,24,24,24                 | 0     |
| 56  | MG   | QA    | 1737 | 1/1   | 0.87 | 0.25 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | RE    | 301  | 1/1   | 0.98 | 0.28 | -    | 1,1,1,1                     | 0     |
| 56  | MG   | RA    | 3269 | 1/1   | 0.95 | 0.40 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3406 | 1/1   | 0.63 | 0.56 | -    | 60,60,60,60                 | 0     |
| 56  | MG   | RB    | 201  | 1/1   | 0.87 | 0.35 | -    | 28,28,28,28                 | 0     |
| 56  | MG   | RA    | 3170 | 1/1   | 0.85 | 0.42 | -    | 26,26,26,26                 | 0     |
| 56  | MG   | RA    | 3321 | 1/1   | 0.96 | 0.27 | -    | 33,33,33,33                 | 0     |
| 56  | MG   | YA    | 3236 | 1/1   | 0.97 | 0.33 | -    | 14,14,14,14                 | 0     |
| 56  | MG   | YA    | 3035 | 1/1   | 0.93 | 0.15 | -    | 29,29,29,29                 | 0     |
| 56  | MG   | QA    | 1676 | 1/1   | 0.96 | 0.31 | -    | 31,31,31,31                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3341 | 1/1   | 0.74 | 0.75 | -    | 71,71,71,71                 | 0     |
| 56  | MG   | QA    | 1740 | 1/1   | 0.93 | 0.51 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3394 | 1/1   | 0.74 | 0.26 | -    | 64,64,64,64                 | 0     |
| 56  | MG   | YA    | 3268 | 1/1   | 0.89 | 0.75 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | RA    | 3221 | 1/1   | 0.97 | 0.28 | -    | 22,22,22,22                 | 0     |
| 56  | MG   | XA    | 1633 | 1/1   | 0.96 | 0.33 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | YA    | 3354 | 1/1   | 0.75 | 0.34 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | QA    | 1663 | 1/1   | 0.81 | 1.39 | -    | 68,68,68,68                 | 0     |
| 56  | MG   | YA    | 3318 | 1/1   | 0.83 | 0.54 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | QA    | 1659 | 1/1   | 0.93 | 0.28 | -    | 25,25,25,25                 | 0     |
| 56  | MG   | RA    | 3017 | 1/1   | 0.92 | 0.12 | -    | 17,17,17,17                 | 0     |
| 56  | MG   | QA    | 1671 | 1/1   | 0.87 | 0.38 | -    | 43,43,43,43                 | 0     |
| 56  | MG   | RA    | 3175 | 1/1   | 0.80 | 0.20 | -    | 46,46,46,46                 | 0     |
| 56  | MG   | RA    | 3024 | 1/1   | 0.98 | 0.47 | -    | 7,7,7,7                     | 0     |
| 56  | MG   | YB    | 206  | 1/1   | 0.88 | 0.13 | -    | 48,48,48,48                 | 0     |
| 56  | MG   | QA    | 1702 | 1/1   | 0.76 | 0.30 | -    | 81,81,81,81                 | 0     |
| 56  | MG   | YB    | 201  | 1/1   | 0.99 | 0.36 | -    | 31,31,31,31                 | 0     |
| 56  | MG   | QA    | 1691 | 1/1   | 0.94 | 0.33 | -    | 20,20,20,20                 | 0     |
| 56  | MG   | QA    | 1709 | 1/1   | 0.82 | 0.42 | -    | 36,36,36,36                 | 0     |
| 56  | MG   | RA    | 3154 | 1/1   | 0.90 | 0.21 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3303 | 1/1   | 0.86 | 0.45 | -    | 69,69,69,69                 | 0     |
| 56  | MG   | YA    | 3342 | 1/1   | 0.82 | 0.52 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | YA    | 3372 | 1/1   | 0.91 | 0.17 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | YA    | 3041 | 1/1   | 0.94 | 0.31 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | QA    | 1711 | 1/1   | 0.91 | 0.37 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3373 | 1/1   | 0.96 | 0.26 | -    | 35,35,35,35                 | 0     |
| 56  | MG   | RA    | 3390 | 1/1   | 0.95 | 0.32 | -    | 49,49,49,49                 | 0     |
| 56  | MG   | YA    | 3387 | 1/1   | 0.87 | 0.21 | -    | 27,27,27,27                 | 0     |
| 56  | MG   | XA    | 1691 | 1/1   | 0.83 | 0.18 | -    | 50,50,50,50                 | 0     |
| 56  | MG   | RA    | 3150 | 1/1   | 0.95 | 0.40 | -    | 40,40,40,40                 | 0     |
| 56  | MG   | RA    | 3348 | 1/1   | 0.98 | 0.34 | -    | 45,45,45,45                 | 0     |
| 56  | MG   | YA    | 3289 | 1/1   | 0.94 | 0.25 | -    | 44,44,44,44                 | 0     |
| 56  | MG   | YA    | 3091 | 1/1   | 0.89 | 0.20 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | YA    | 3445 | 1/1   | 0.97 | 0.10 | -    | 19,19,19,19                 | 0     |
| 56  | MG   | RQ    | 201  | 1/1   | 0.82 | 0.40 | -    | 23,23,23,23                 | 0     |
| 56  | MG   | YA    | 3312 | 1/1   | 0.97 | 0.39 | -    | 63,63,63,63                 | 0     |
| 56  | MG   | QA    | 1735 | 1/1   | 0.90 | 0.56 | -    | 66,66,66,66                 | 0     |
| 56  | MG   | RA    | 3179 | 1/1   | 0.96 | 0.40 | -    | 30,30,30,30                 | 0     |
| 56  | MG   | YA    | 3214 | 1/1   | 0.88 | 0.71 | -    | 53,53,53,53                 | 0     |
| 56  | MG   | YA    | 3263 | 1/1   | 0.77 | 0.34 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3440 | 1/1   | 0.83 | 0.30 | -    | 62,62,62,62                 | 0     |
| 56  | MG   | RA    | 3346 | 1/1   | 0.93 | 0.34 | -    | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56  | MG   | YA    | 3461 | 1/1   | 0.93 | 0.15 | -    | 37,37,37,37                 | 0     |
| 56  | MG   | RA    | 3326 | 1/1   | 0.72 | 0.42 | -    | 56,56,56,56                 | 0     |
| 56  | MG   | XA    | 1753 | 1/1   | 0.94 | 0.28 | -    | 70,70,70,70                 | 0     |
| 56  | MG   | YA    | 3275 | 1/1   | 0.94 | 0.34 | -    | 41,41,41,41                 | 0     |
| 56  | MG   | YA    | 3316 | 1/1   | 0.98 | 0.11 | -    | 30,30,30,30                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.